

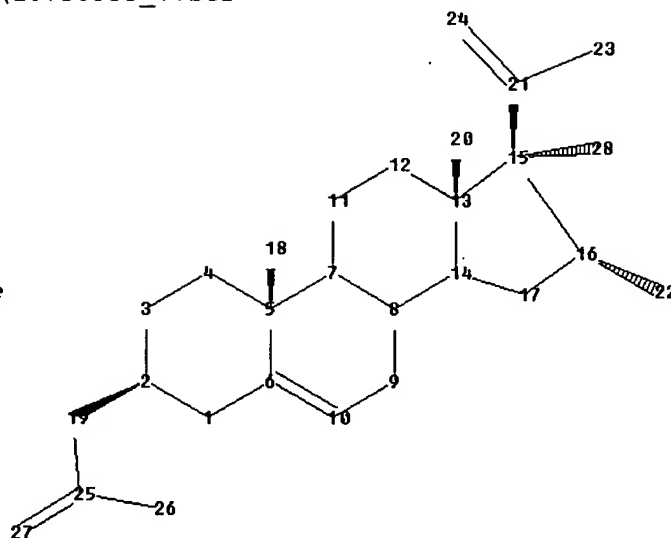
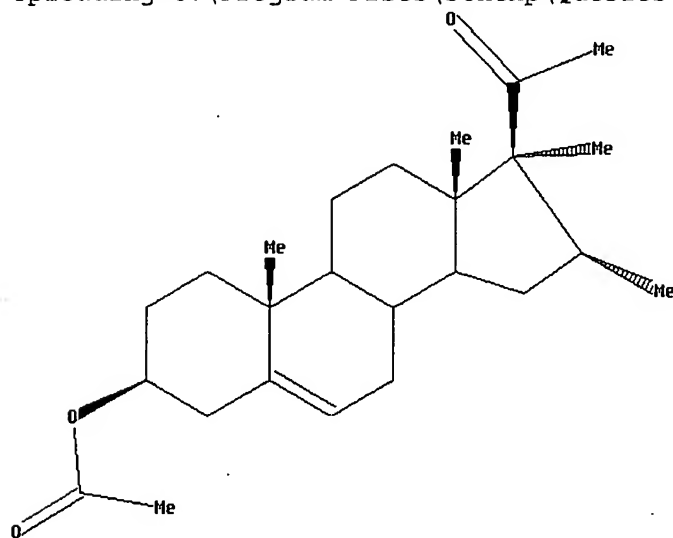
FILE 'HOME' ENTERED AT 10:17:43 ON 08 JAN 2007

=> file registry

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Uploading C:\Program Files\Stnexp\Queries\10758335_V.str

Compound V



chain nodes :

18 19 20 21 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-19 5-18 13-20 15-21 15-28 16-22 19-25 21-23 21-24 25-26 25-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
12-13 13-14 13-15 14-17 15-16 16-17 19-25 21-24 25-27

exact bonds :

5-18 13-20 15-21 15-28 16-22 21-23 25-26

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

Stereo Bonds:

18-5 (Single Wedge).
19-2 (Single Wedge).
20-13 (Single Wedge).
21-15 (Single Wedge).
22-16 (Single Hash).
28-15 (Single Hash).

Stereo Chiral Centers:

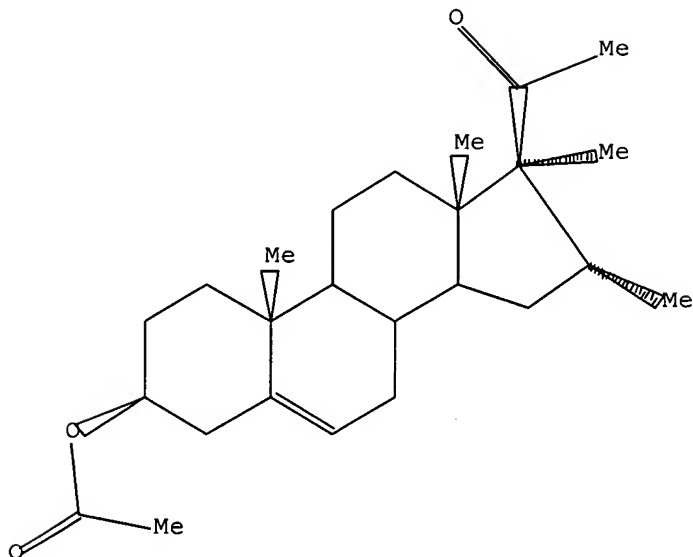
2 (Parity=Odd)

Stereo RSS Sets:

L1 STRUCTURE UPLOADED

L1 HAS NO ANSWERS

L1	STR
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=> s 11

SAMPLE SCREEN SEARCH COMPLETED - 111 TO ITERATE

0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTED ITERATIONS: 1588 TO 2852

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA.SSS SAM L1

FULL SEARCH INITIATED 10:18:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

1 ANSWERS

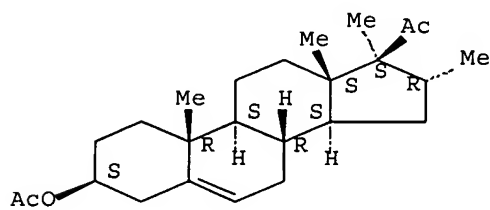
SEARCH TIME: 00.00.01

L3 1 SEA EXA FUL L1

=> d 13

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 13116-52-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pregn-5-en-20-one, 3 β -hydroxy-16 α ,17-dimethyl-, acetate (7CI,
8CI)
OTHER NAMES:
CN 16 α ,17 α -Dimethylpregnenolone acetate
FS STEREOSEARCH
MF C25 H38 O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file medline, caplus, wpids, uspatfull

=> s 13

SAMPLE SEARCH INITIATED 10:18:56 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 62
PROJECTED ANSWERS: 0 TO 0

L4 9 L3

=> d 14 1-9 ibib, abs, hitstr

L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:32514 CAPLUS Full-text

DOCUMENT NUMBER: 138:304436

TITLE: Synthesis of 3 β -hydroxy-16 α ,17 α ,21-trimethylpregn-5-en-20-one

AUTHOR(S): Wang, Li; Zhu, Cui-Hong; Zhang, Xiang-Wen; Mi, Zhen-Tao

CORPORATE SOURCE: School of Chemical Engineering and Technology, Tianjin University, Tianjin, 300072, Peop. Rep. China

SOURCE: Yingyong Huaxue (2002), 19(12), 1189-1191

CODEN: YIHUED; ISSN: 1000-0518

PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 138:304436

AB Title compound was synthesized from 3 α -acetoxypregna-5,16-dien-20-one via methylation with methylmagnesium bromide followed with Me iodide giving product with yield 78%. LHDMS ([$(\text{CH}_3)_3\text{Si}$] 2NLi) and LDA ([$(\text{CH}_3)_2\text{CH}$] 2NLi) were chosen as proper reagents for 21-position alkylation. The product was characterized by elemental anal., ^1H NMR, MS and IR.

IT 13116-52-4P

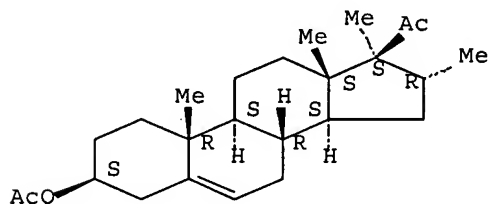
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of 3 β -hydroxy-16 α ,17 α ,21-trimethylpregn-5-en-20-one)

RN 13116-52-4 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:221159 CAPLUS Full-text

DOCUMENT NUMBER: 136:257280

TITLE: Methods and compositions that affect melanogenesis

INVENTOR(S): Orlow, Seth J.; Hall, Andrea; Manga, Prashiela

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U. S. Ser. No. 599,487.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR

EP 1383474	A2	20040128	EP 2002-776548	20020408
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420

PRIORITY APPLN. INFO.:

US 1999-141563P	P	19990629
US 2000-599487	A2	20000623
US 2001-827428	A	20010406
WO 2002-US11067	W	20020408
US 2004-758335	A3	20040115

AB The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

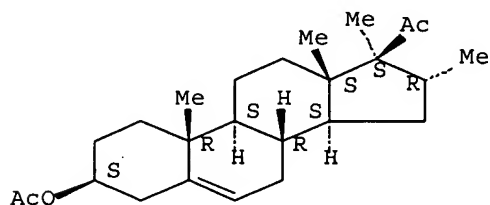
IT 13116-52-4

RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. that affect melanogenesis)

RN 13116-52-4 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:456114 CAPLUS Full-text

DOCUMENT NUMBER: 97:56114

TITLE: Alkylated steroids. Part 5. Formation of 17 β -acetylenic steroids from hindered 20-oxo compounds via Grignard derived enolates

AUTHOR(S): Logan, Robert T.; Roy, Robert G.; Woods, Gilbert F.

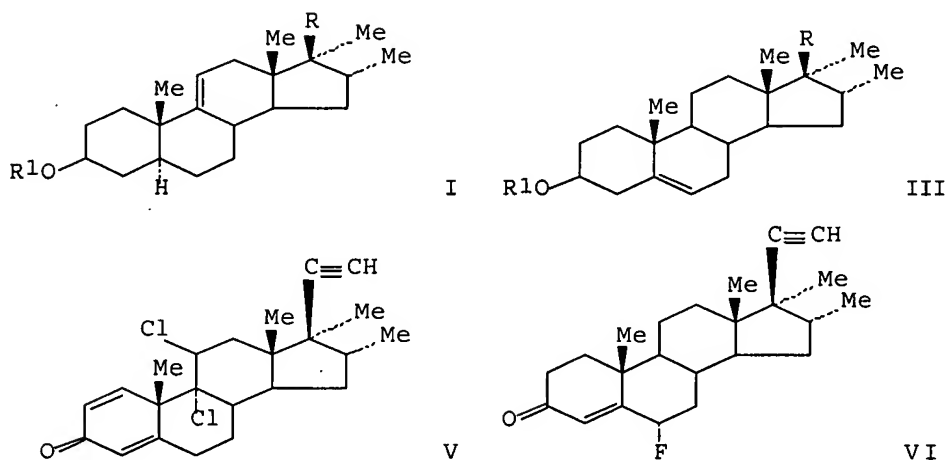
CORPORATE SOURCE: Organon Sci. Dev. Group, Organon Lab. Ltd., Newhouse,
ML1 5SH, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)
(1982), (4), 1079-84
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Pregnynynol I ($R = \text{C.tplbond.CH}$, $R_1 = \text{H}$) (II) was prepared by treatment of I ($R = \text{CO}_2\text{Me}$, $R_1 = \text{Ac}$; $R = \text{COMe}$, COCH_2Br , $R_1 = \text{H}$) with MeMgX ($X = \text{Cl}$, Br) in C_6H_6 or THF followed by refluxing in anisole. III ($R = \text{COMe}$, $R_1 = \text{Ac}$) similarly gave III ($R = \text{C.tplbond.CH}$, $R_1 = \text{H}$) (IV). The mechanisms of these reactions is discussed in relation to the steric hindrance of the 16- and 17-Me groups. II and IV were converted to pregnenynones V and VI, resp., in 3 and 5 steps, resp.

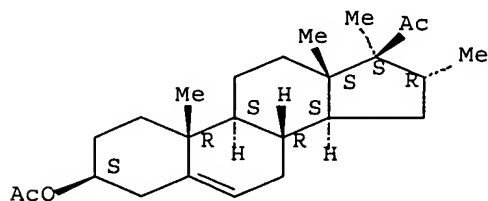
IT 13116-52-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with halomethane)

RN 13116-52-4 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:35625 CAPLUS Full-text

DOCUMENT NUMBER: 96:35625

TITLE: Alkylated steroids. Part 3. The 21-alkylation of 20-oxopregnanes and synthesis of a novel antiinflammatory 16 α ,17 α ,21-trimethyl steroid (Org 6216)

AUTHOR(S): Cairns, James; Logan, Robert T.; McGarry, George; Roy, Robert G.; Stevenson, Donald F. M.; Woods, Gilbert F.

CORPORATE SOURCE: Organon Sci. Dev. Group, Organon Lab. Ltd., Newhouse, ML1 5SH, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1981), (8), 2306-16

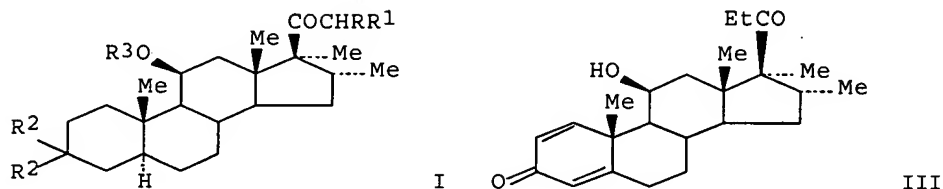
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:35625

GI



AB The alkylation at C-21 of steroidal derivs. via the Li 20(21)-enolate is described, and a number of C-21 alkylpregnane derivs. were prepared E.g., reaction of the pregnane acetal I (R = R₁ = H, R₂ = OMe, R₃ = Ac) with LiN(CHMe₂)₂ (THF, -50 to -45°) then Me iodide (room temperature, 30 min) followed by deprotection gave 85% I (R = Me, R₁ = H, R₂R₂ = O, R₃ = COEt) (II). Sequential bromination, dehydrobromination, oxidation, and hydrolysis of II gave methylpregnadienone (Org 6216) III in 75% overall yield.

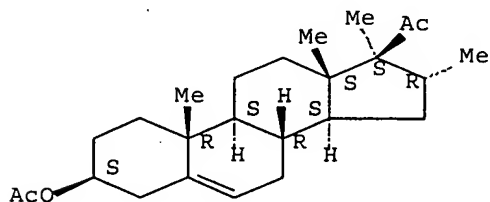
IT 13116-52-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

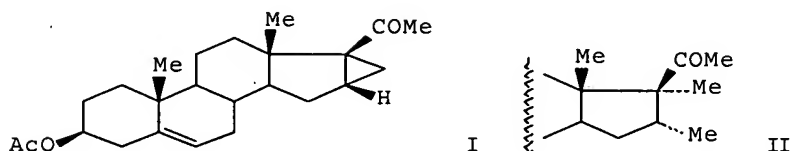
RN 13116-52-4 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1981:604267 CAPLUS Full-text
 DOCUMENT NUMBER: 95:204267
 TITLE: Transformed steroids. 122. Functionalization of the carbon-17 center of 2-keto steroids via reduction cleavage of the 16 α ,17 α -cyclopropane ring
 AUTHOR(S): Kamernitskii, A. V.; Kulikova, L. E.; Levina, I. S.
 CORPORATE SOURCE: Inst. Org. Khim., Moscow, USSR
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (6), 1384-7
 CODEN: IASKA6; ISSN: 0002-3353
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB Reductive ring cleavage of 16,17-cyclopropano-20-oxopregnanes by Li in NH₃(l) and subsequent treatment with electrophilic reagents resulted in regiospecific and stereospecific functionalization of C-17. Thus, treatment of cyclopropanopregnene I with Li in NH₃(l) and then successive treatment with MeI, aqueous NH₄Cl, and Ac₂O in pyridine gave methylpregnenone II.

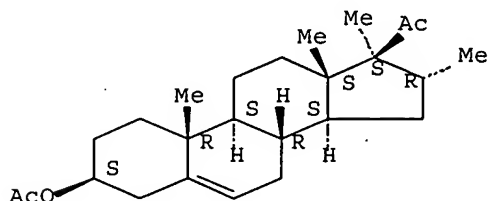
IT 13116-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 13116-52-4 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-
 (9CI) (CA INDEX NAME)

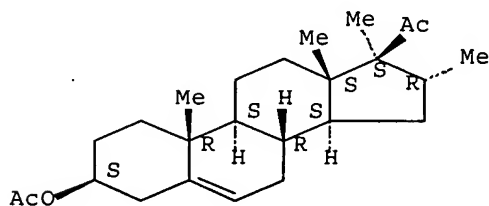
Absolute stereochemistry.



L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1973:148118 CAPLUS Full-text
 DOCUMENT NUMBER: 78:148118
 TITLE: Preparation of formates of isomeric pregnane 5,6-bromohydrins

AUTHOR(S): Bayunova, V. I.; Akalaev, A. N.; Pakhomov, V. P.; Grinenko, G. S.
 CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
 SOURCE: Khimiya Prirodnikh Soedinenii (1973), 9(1), 39-45
 CODEN: KPSUAR; ISSN: 0023-1150
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI For diagram(s), see printed CA Issue.
 AB Pregnenolone acetate was treated with aqueous HOBr in DMF to yield bromopregnanediol formates I and II and pregnanetriol acetate III (R = R1 = H). Similarly, 16,17-dimethyl-pregnenolone acetate (IV) gave I and II (R = R1 = Me); and 16,17-epoxypregnenolone acetate yielded I, II (RR1 = O) and 5 α -bromo-16,17-epoxy-6 β -hydroxypregnenolone 3-acetate. IV was treated with aqueous HOBr in EtOAc to give the bromohydroxy-pregnanones V and VI (R = R1 = Me). The 5,6-bromohydrin compds. yielded 5,6-epoxy derivs. when treated with KOAc or K₂CO₃.
 IT 13116-52-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with hypobromous acid and DMF)
 RN 13116-52-4 CAPLUS
 CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-(9CI) (CA INDEX NAME)

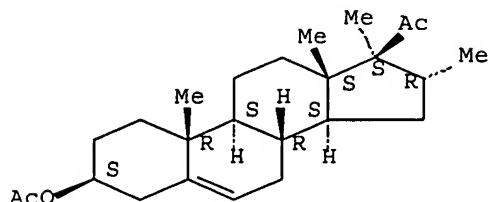
Absolute stereochemistry.



L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1967:444004 CAPLUS Full-text
 DOCUMENT NUMBER: 67:44004
 TITLE: Synthesis of 17-bromo-16 α -methylprogesterones
 AUTHOR(S): Reimann, Hans; Sarre, Olga Z.
 CORPORATE SOURCE: Schering Corp., Bloomfield, NJ, USA
 SOURCE: Journal of Organic Chemistry (1967), 32(7), 2321-4
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB In situ bromination of 16 α -methylpregnane 20-magnesium enolates gives a mixture of the 17 α -bromo- and 17 β -bromo-20-oxo derivs. Utilizing this reaction, 17 α -bromo-16 α -methylprogesterone (II) and 17 β -bromo-16 α -methyl-17-isoprogerone (I) were prepared from 16-dehydropregnenolone acetate (III). 21 references.
 IT 13116-52-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 13116-52-4 CAPLUS
 CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:455330 CAPLUS Full-text

DOCUMENT NUMBER: 59:55330

ORIGINAL REFERENCE NO.: 59:10161f-h,10162a

TITLE: Gas chromatography of selected pregnenes and pregnanes

AUTHOR(S): Nelson, J. P.

CORPORATE SOURCE: Gen. Mills Res. Labs., Minneapolis, MN

SOURCE: Journal of Gas Chromatography (1963), 1(3), 27-9

CODEN: JGCRAJ; ISSN: 0096-2686

DOCUMENT TYPE: Journal

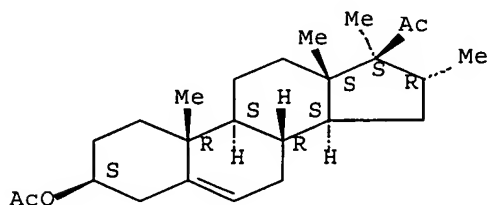
LANGUAGE: Unavailable

AB Relative retention times on SE-30 silicone gum and on QF-1-0065 fluorinated silicone both at 221° are given: (SE-30, QF-1-0065) for 5 β -16-pregnene-3 β -ol-20-one (0.55, 2.17) and acetate (0.75, 3.78), 16-dehydropregnenolone (0.58, 2.42) and acetate (0.86, 4.04), pregnenolone (0.63, 2.76) and acetate (0.94, 4.81), 16 α -methylpregnenolone (0.64, 2.64) and acetate (0.93, 4.16), 16 α ,17 α -epoxypregnenolone (0.66, 2.96), 16-methyl-16-dehydropregnenolone (0.74, 3.10) and acetate (1.12, 5.31), 5 β -pregnane-3 β ,17 α -diol-20-one (0.86, 3.45), 17 α -hydroxypregnenolone (0.88, 4.13) and acetate (1.25, 6.93), 5 α ,6 α -epoxy-5 α -pregnan-3 β -ol-20-one (0.92, 5.88) and acetate (1.41, 11.4), 6 β ,16 α -dimethyl-5 α -pregnane-3 β ,5 α -diol-20-one (1.29, 6.41) and acetate (1.29, 10.8), 6 β -methyl-5 α -pregnane-3 β ,5 α -diol-20-one (1.31, 7.13), 16 α ,17 α -dimethylpregnenolone acetate (1.00, 5.10), 6,16 α -dimethylpregnenolone acetate (1.07, 4.20), 16 β -methylpregnenolone acetate (1.08, 4.40), 5 β ,6 β -epoxypregnan-3 β -ol-20-one 3-acetate (1.23, decompose), 5 α ,6 α -epoxy-16-pregnen-3 β -ol-20-one 3-acetate (1.32, 10.5), 5 α -pregnane-3 β ,17 α -diol-20-one 3-acetate (1.32, 7.42), 5 α ,6 α :16 α ,17 α -diepoxy-5 α -pregnan-3 β -ol-20-one-3 acetate (15.0, not eluted), 20,20-ethylenedioxyregnenolone acetate (1.79, 4.30), 16 α -methyl-20,20-ethylenedioxyregnenolone acetate (1.85, 4.20), 16 α -methyl-5 α ,6 α -epoxy-5 α -pregnane-3 β ,17 α -diol-20-one 3-acetate (2.44, not eluted), 5 α ,6 α -epoxy-20,20-ethylenedioxy-5 α -pregnan-3 β -ol 3-acetate (2.80, 11.5), 5 α ,6 α -epoxy-16 α -methyl-20,20-ethylenedioxy-5 α -pregnan-3 β -ol 3-acetate (2.85, 10.7). Relative retention times are given by the formula $x = y + a + b + \dots + n$ where x is the time of the substance to be calculated, y that of the parent substance, and a , b , ... n , the contributions of substituent groups as follows (acetates): 16 α -methyl (-0.01, -0.65), Δ 16 (-0.08, -0.77), 16 α ,17 α -epoxy (0.06, 0.29), 16 β -methyl (0.14, -0.41), 17 α -hydroxy (0.31, 2.12), 5 α ,6 α -epoxy (0.48, 6.59), 20,29-ethylenedioxy (0.85, -0.51), 6-methyl (0.14, 0.04); (alcohols): 16 α -methyl (0.01, -0.12), Δ 16 (-0.05, -0.34), 17 α -hydroxy (0.25, 1.37), 5 α ,6 α -epoxy (0.29, 3.12). Results are within 1.5% of exptl. values,

except in the case of 5 α ,6 α -epoxy-20,20-ethylenedioxy- 5 α -pregnan-3 β -ol 3-acetate on SE-30 which is 23% in error.

IT 13116-52-4, Pregn-5-en-20-one, 3 β -hydroxy-16 α ,17-dimethyl-, acetate
(chromatography of)
RN 13116-52-4 CAPLUS
CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 9 OF 9 USPATFULL on STN

ACCESSION NUMBER: 2002:60938 USPATFULL Full-text
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
Hall, Andrea, New York, NY, UNITED STATES
Manga, Prashiela, New York, NY, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-141563P	19990629 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	92	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	4216	

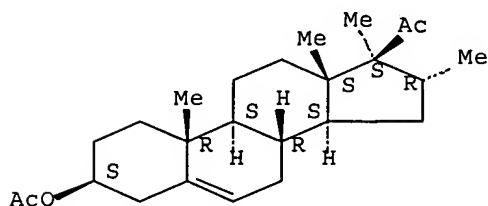
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 13116-52-4
 (methods and compns. that affect melanogenesis)
 RN 13116-52-4 USPATFULL
 CN Pregn-5-en-20-one, 3-(acetyloxy)-16,17-dimethyl-, (3 β ,16 α)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

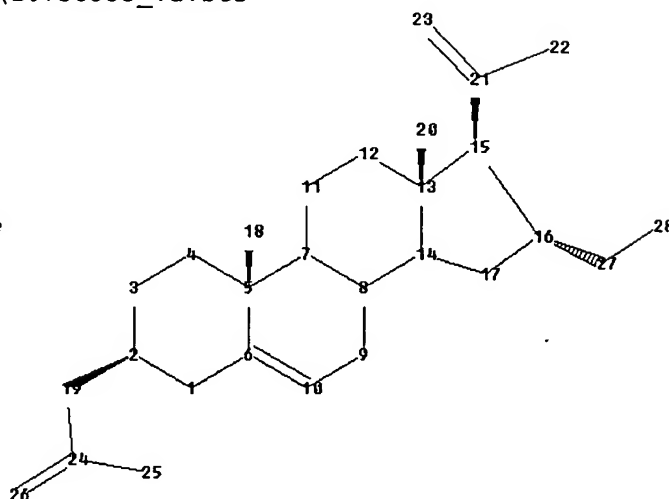
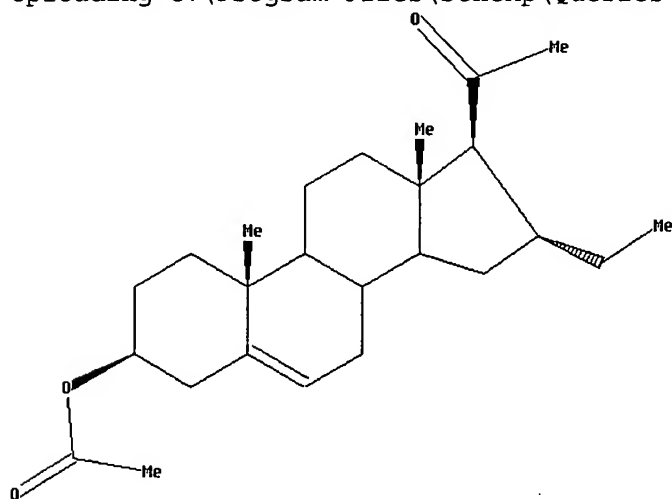


=> file registry

=>

Uploading C:\Program Files\Stnexp\Queries\10758335_VI.str

COMPOUND VI



chain nodes :

18 19 20 21 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-19 5-18 13-20 15-21 16-27 19-24 21-22 21-23 24-25 24-26 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
 13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
 12-13 13-14 13-15 14-17 15-16 16-17 19-24 21-23 24-26

exact bonds :

5-18 13-20 15-21 16-27 21-22 24-25 27-28

Match level :

Stereo Bonds:

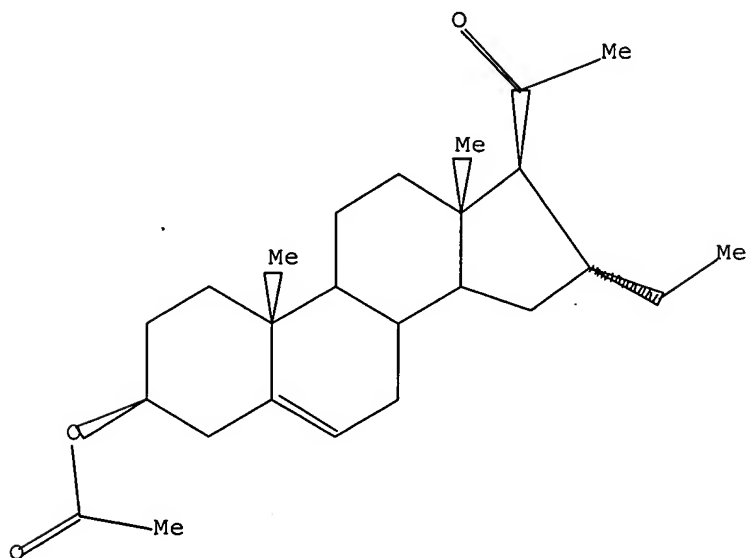
Stereo Chiral Centers:

Stereo RSS Sets:

=> d 15

L5 HAS NO ANSWERS

L5 STR



=> s 15

SAMPLE SEARCH INITIATED 10:20:55 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 exa full

FULL SEARCH INITIATED 10:21:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 27 TO ITERATE

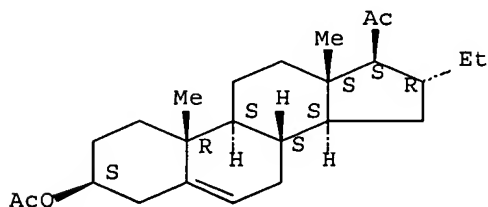
100.0% PROCESSED 27 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L7 1 SEA EXA FUL L5

=> d 17

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 5297-33-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pregn-5-en-20-one, 16 α -ethyl-3 β -hydroxy-, acetate (6CI, 7CI, 8CI)
FS STEREOSEARCH
MF C25 H38 O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file medline, caplus, wpids, uspatfull

=> s 17

SAMPLE SEARCH INITIATED 10:21:26 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 62
PROJECTED ANSWERS: 0 TO 0

L8 8 L7

=> d 18 1-8 ibib, abs, hitstr

L8 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:221159 CAPLUS Full-text **APPLICANT**
DOCUMENT NUMBER: 136:257280
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J.; Hall, Andrea; Manga, Prashiela
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U. S.
Ser. No. 599,487.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR			
EP 1383474	A2	20040128	EP 2002-776548	20020408
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420
PRIORITY APPLN. INFO.:			US 1999-141563P	P 19990629
			US 2000-599487	A2 20000623
			US 2001-827428	A 20010406
			WO 2002-US11067	W 20020408
			US 2004-758335	A3 20040115

AB The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of

melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

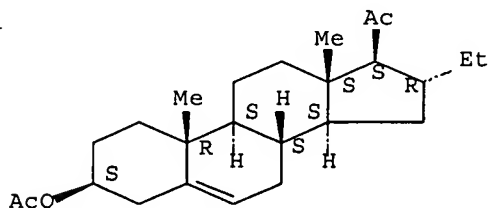
IT 5297-33-6

RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. that affect melanogenesis)

RN 5297-33-6 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:517611 CAPLUS Full-text

DOCUMENT NUMBER: 119:117611

TITLE: Methylation or ethylation agents comprising trimethylaluminum, tiethylaluminum, or diethyl zinc and catalytic copper compounds for conjugate addition reactions

INVENTOR(S): Westermann, Juergen; Nickisch, Klaus

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 534582	A1	19930331	EP 1992-250276	19920928
EP 534582	B1	19970108		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
DE 4132755	A1	19930401	DE 1991-4132755	19910927
CA 2120004	A1	19930401	CA 1992-2120004	19920928
CA 2120004	C	20060110		
WO 9306066	A1	19930401	WO 1992-EP2227	19920928
W: CA, JP, US				
JP 06511485	T	19941222	JP 1992-505811	19920928
AT 147401	T	19970115	AT 1992-250276	19920928
ES 2098442	T3	19970501	ES 1992-250276	19920928
JP 3279564	B2	20020430	JP 1993-505811	19920928
US 5908944	A	19990601	US 1994-211230	19940930
PRIORITY APPLN. INFO.:			DE 1991-4132755	A 19910927
			WO 1992-EP2227	W 19920928
OTHER SOURCE(S): CASREACT 119:117611; MARPAT 119:117611				

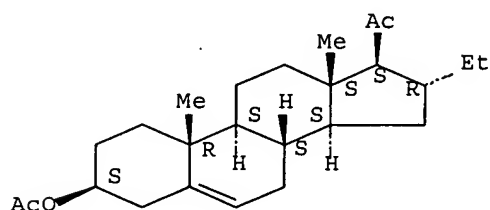
AB Ethylating or methylating agents consist of Me₃Al, Me₂Zn or Et₃Al combined with catalytic quantities of ≥ 1 Cu(I) and/or Cu(II) compound. Thus, a mixture of androsta-1,4-dien-3,17-dione and CuBr in dioxane was treated with Me₃Al in PhMe at $\leq 35^\circ$ to give 77% 1 α -methylandrosta-4-en-3,17-dione.

IT 5297-33-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, via conjugate addition reaction using triethylaluminum and cuprous bromide)

RN 5297-33-6 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:225091 CAPLUS Full-text

DOCUMENT NUMBER: 104:225091

TITLE: Synthesis of 16 α -ethyl-21-hydroxy-19-norpregn-4-ene-3,20-dione

AUTHOR(S): Zeelen, F. J.; Van den Broek, A. J.

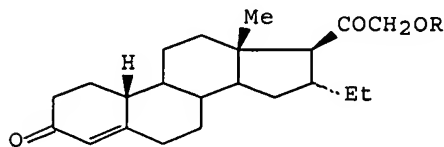
CORPORATE SOURCE: Organon Sci. Dev. Group, Oss, 5340 BH, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1985), 104(9), 239-42
 CODEN: RTCPA3; ISSN: 0034-186X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The title compound I (R = H) was prepared from 3 β -acetoxypregna-5,16-dien-20-one in 11 steps and esterified by acyl chlorides to give I (R = hexanoyl, heptanoyl, decanoyl, dodecanoyl, hexadecanoyl, PhCH₂CH₂CO). I (R = H) possessed progestational activity 36 times that of progesterone, and I (R = dodecanoyl) was active for months after a single injection in mammals.

IT 5297-33-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

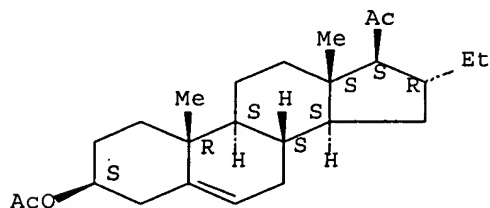
(Reactant or reagent)

(preparation and hydroxybromination of)

RN 5297-33-6 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:425847 CAPLUS Full-text

DOCUMENT NUMBER: 81:25847

TITLE: Transformed steroids. LV. Reaction of
trialkylboranes with Δ^{16-20} -keto steroids

AUTHOR(S): Akhrem, A. A.; Levina, I. S.; Titov, Yu. A.; Khripach,
V. A.; Bubnov, Yu. N.; Mikhailov, B. M.

CORPORATE SOURCE: USSR

SOURCE: Zhurnal Obshchei Khimii (1973), 43(11), 2565-71
CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB 3 β -Acetoxypregna-5,16-dien-20-one (I) reacted with R₃B (R = Et, Bu, Me₂CHCH₂) in refluxing THF containing H₂O and then with alkaline H₂O₂ to give 10.2-32% yields of the corresponding pregnenones II and 32-4% yields of (tetrahydrofuran-5-yl)pregnenone III. Similar reaction of I with Bu₃B in Me₂CHOH gave II (R = Bu) and (hydroxyisopropyl)pregnenone IV. The configuration at C-16 was determined by CD spectroscopy. II (R = Bu, Me₂CHCH₂) were also prepared by reaction of I with RMgBr in the presence of CuBr.

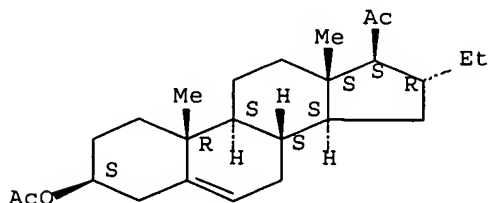
IT 5297-33-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5297-33-6 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:36099 CAPLUS Full-text

DOCUMENT NUMBER: 64:36099

ORIGINAL REFERENCE NO.: 64:6715d-f

TITLE: The Beckmann rearrangement of pregna-5,16-dien-3 β -ol-20-one acetate with boron trifluoride

AUTHOR(S): Romo, J.; de Vivar, A. Romo

CORPORATE SOURCE: Univ. Anatomia, Mexico, D.F.

SOURCE: Revista de la Sociedad Quimica de Mexico (1962), 6(3), 77-86

CODEN: RSQMAN; ISSN: 0583-7693

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

AB The Beckmann rearrangement of 20-acetoximinopregna-5,16-dien-3 β -ol acetate catalyzed with BF₃ in benzene as solvent gave dehydroepiandrosterone as final product. However, when the reaction was performed using as solvent Ac₂O, 17 β -methyl-18-norisopregna-5,13-diene-3 β ,16 α -diol-20-one diacetate (I) and 16-acetyl-17-acetamidoandrosta-5,16-dien-3 β -ol (II) were obtained. I had λ 5.80 μ with inflection in 5.88 μ . I formed an oxime and gave a diepoxide when treated with perbenzoic acid. II was shown to contain N. For further identification several derivs. of both I and II were prepared and identified. The reaction is useful to prepare androstane derivs. starting from Δ 16-20-ketones.

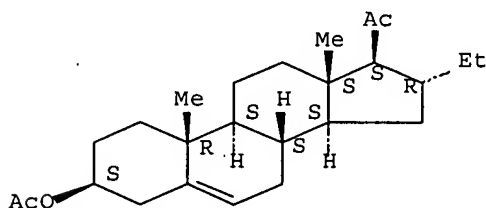
IT 5297-33-6P, Pregn-5-en-20-one, 16 α -ethyl-3 β -hydroxy-, acetate

RL: PREP (Preparation)
(preparation of)

RN 5297-33-6 CAPLUS

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1961:8299 CAPLUS Full-text

DOCUMENT NUMBER: 55:8299

ORIGINAL REFERENCE NO.: 55:1697a-c

TITLE: Beckmann rearrangement of the acetoxime of 5,16-pregnadien-3 β -ol-20-one acetate with boron trifluoride

AUTHOR(S): Romo, J.; de Vivar, A. Romo

CORPORATE SOURCE: Univ. Mexico, Mexico City

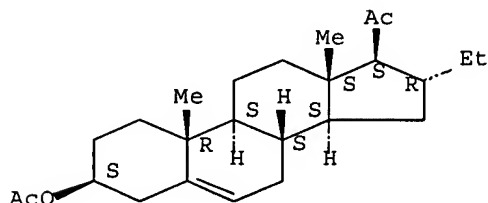
SOURCE: Journal of the American Chemical Society (1959), 81,

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:8299

AB Beckmann rearrangement of 3 β -acetoxy-5,16-pregnadien-20-one acetoxime with BF₃-Et₂O in benzene yielded dehydroepiandrosterone acetate, whereas in Ac₂O the rearrangement followed a different course and two products were isolated: 17 β -methyl-18-nor-5,13(14)-isopregnadiene-3 β , 16 α -diol-20-one diacetate (I) and 16-acetyl-17-acetamido-5,16-androstadien-3 β -ol acetate (II). Several derivs. of these compds. were prepared in the process of establishing their structure. LiAlH₄ reduction of I afforded the 3,16,20-triol, m. 202-204°, [α]_D -207°. The oxo group in I was eliminated by hydrogenolysis of the cycloethylene mercaptol, m. 137-40°, [α]_D -108°, whereupon the diacetate, m. 123-4°, [α]_D -176°, was obtained. KHCO₃ saponification of the diacetate gave the monoacetate which, on Oppenauer oxidation, afforded the Δ^4 -3-ketone. II was hydrolyzed with KOH to remove the acetate groups and the latter benzoylated with BzCl in pyridine to give the dibenzoate, m. 279-81°, [α]_D -44°. Benzoylation by the Schotten-Baumann method gave the monobenzoate (III), m. 218-20°, [α]_D -51°. Oppenauer oxidation of III yielded 16-acetyl-17-benzamido-4,16-androstadien-3-one, m. 221-2°, [α]_D 94°.

IT	5297-33-6P, Pregn-5-en-20-one, 16 α -ethyl-3 β -hydroxy-, acetate RL: PREP (Preparation) (preparation of)
RN	5297-33-6 CAPLUS
CN	Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 7 OF 8 USPATFULL on STN
ACCESSION NUMBER: 2002:60938 USPATFULL Full-text
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
Hall, Andrea, New York, NY, UNITED STATES
Manga, Prashiela, New York, NY, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

NUMBER DATE

PRIORITY INFORMATION: US 1999-141563P 19990629 (60)
 DOCUMENT TYPE: Utility
 FILE SEGMENT: APPLICATION
 LEGAL REPRESENTATIVE: ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109
 NUMBER OF CLAIMS: 92
 EXEMPLARY CLAIM: 1
 NUMBER OF DRAWINGS: 19 Drawing Page(s)
 LINE COUNT: 4216
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

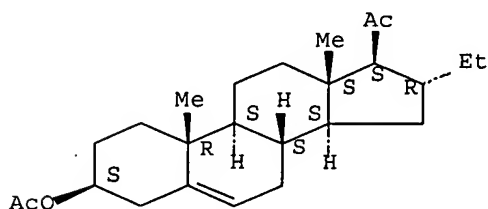
IT 5297-33-6

(methods and compns. that affect melanogenesis)

RN 5297-33-6 USPATFULL

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 8 OF 8 USPATFULL on STN

ACCESSION NUMBER: 1999:63417 USPATFULL Full-text

TITLE: Methylation or ethylation agent and process for
 1,4-addition of a methyl or ethyl group to an α ,
 β -unsaturated keto compound

INVENTOR(S): Westermann, Jurgen, Berlin, Germany, Federal Republic
 of

PATENT ASSIGNEE(S): Nickisch, Klaus, Berlin, Germany, Federal Republic of
 Schering Aktiengesellschaft, Germany, Federal Republic
 of (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5908944		19990601
	WO 9306066		19930401
APPLICATION INFO.:	US 1994-211230		19940930 (8)
	WO 1992-EP2227		19920928
			19940930 PCT 371 date

	NUMBER	DATE
PRIORITY INFORMATION:	DE 1991-4132755	19910927
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Dees, Jose G.	
ASSISTANT EXAMINER:	Pryor, Alton	
LEGAL REPRESENTATIVE:	Millen, White, Zelano, & Branigan, P.C.	
NUMBER OF CLAIMS:	21	
EXEMPLARY CLAIM:	1	
LINE COUNT:	980	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention describes a new methylation or ethylation agent containing trimethyl aluminum or dimethyl zinc or triethyl aluminum as methyl or ethyl source, which additionally contains catalytic amounts of one or more copper(I) and/or copper(II) compounds as well as a process for the 1,4-addition of a methyl or ethyl group to an α,β -unsaturated or an α,β -double unsaturated ketone or an α,β -unsaturated aldehyde using the agent according to the invention.

By using only catalytic amounts of copper and a CKW (chlorinatedhydrocarbon)-free reaction medium, the new methylation/ethylation agent/process is distinguished by its environmental compatibility and it is, for example, suitable for the production of initial products for the synthesis of biologically effective compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

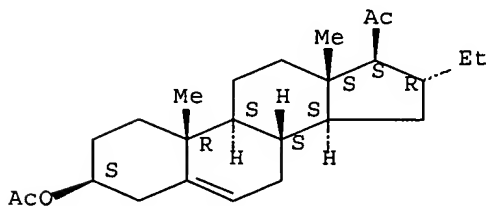
IT 5297-33-6P

(preparation of, via conjugate addition reaction using triethylaluminum and cuprous bromide)

RN 5297-33-6 USPATFULL

CN Pregn-5-en-20-one, 3-(acetyloxy)-16-ethyl-, (3 β ,16 α)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

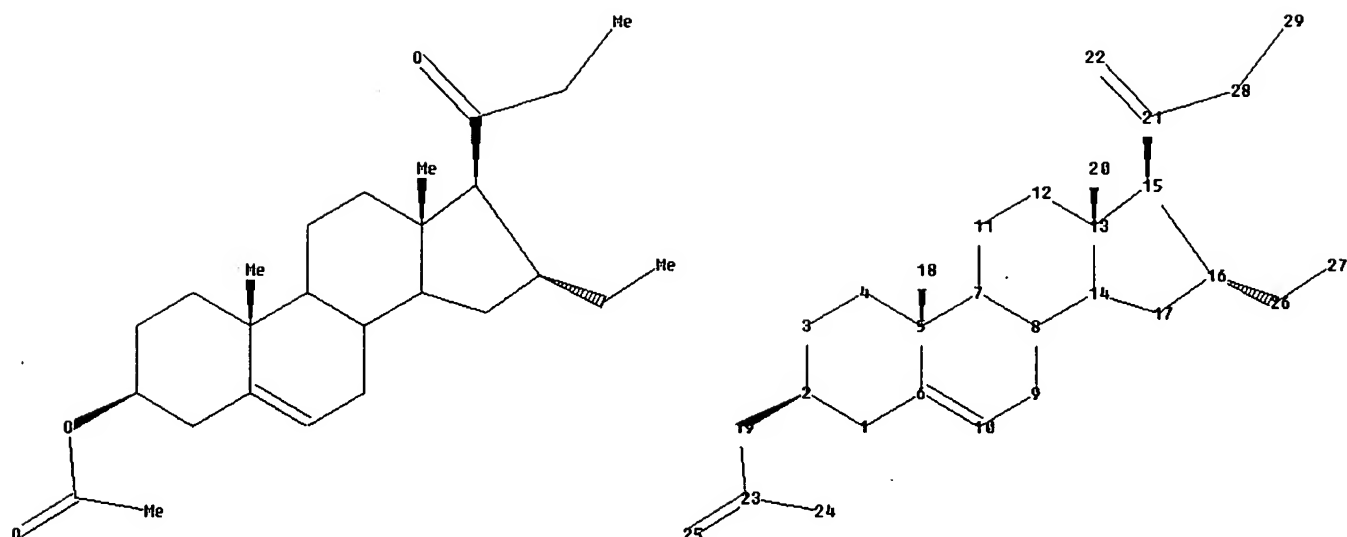


=> file registry

Compound VII

=>

Uploading C:\Program Files\Stnexp\Queries\10758335_VII.str



chain nodes :

18 19 20 21 22 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-19 5-18 13-20 15-21 16-26 19-23 21-22 21-28 23-24 23-25 26-27 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
12-13 13-14 13-15 14-17 15-16 16-17 19-23 21-22 23-25

exact bonds :

5-18 13-20 15-21 16-26 21-28 23-24 26-27 28-29

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS

Stereo Bonds:

18-5 (Single Wedge).
19-2 (Single Wedge).
20-13 (Single Wedge).
21-15 (Single Wedge).
26-16 (Single Hash).

Stereo Chiral Centers:

2 (Parity=Odd)
5 (Parity=Even)
13 (Parity=Even)
15 (Parity=Odd)
16 (Parity=Even)

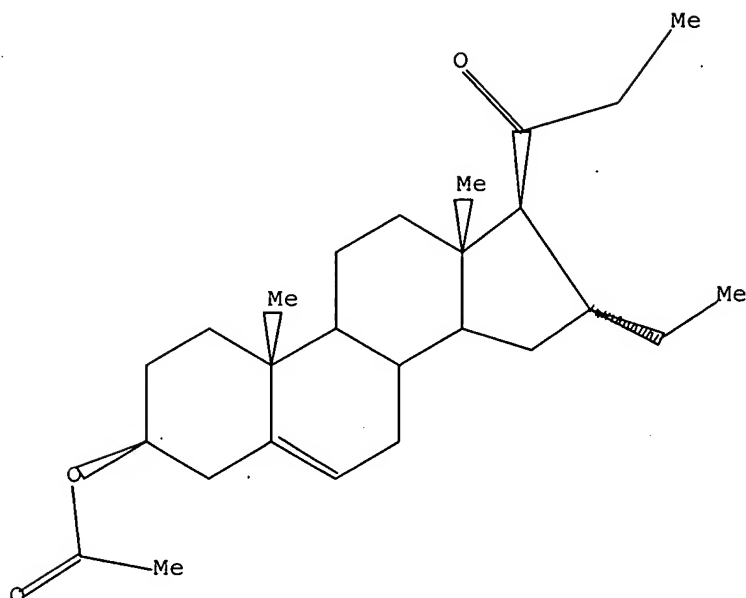
Stereo RSS Sets:

Type=Relative (Default). 5 Nodes= 2 5 13 15 16
L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19 exa full

FULL SEARCH INITIATED 10:23:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 27 TO ITERATE

100.0% PROCESSED 27 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L10 1 SEA EXA FUL L9

=> file medline, caplus, wpids, uspatfull

=> s 110

SAMPLE SEARCH INITIATED 10:23:20 FILE 'WPIDS'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1 TO 40

PROJECTED ANSWERS: 0 TO 0

L11

3 L10

=> d 111 1-3 ibib, abs, hitstr

L11 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:221159 CAPLUS Full-text

APPLICANT

DOCUMENT NUMBER: 136:257280

TITLE: Methods and compositions that affect melanogenesis

INVENTOR(S): Orlow, Seth J.; Hall, Andrea; Manga, Prashiela

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U. S.
Ser. No. 599,487.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1383474	A2	20040128	EP 2002-776548	20020408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420
PRIORITY APPLN. INFO.:				
			US 1999-141563P	P 19990629
			US 2000-599487	A2 20000623
			US 2001-827428	A 20010406
			WO 2002-US11067	W 20020408
			US 2004-758335	A3 20040115

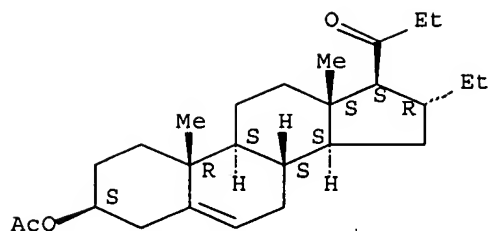
AB The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

IT 16321-62-3
RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. that affect melanogenesis)

RN 16321-62-3 CAPLUS

CN 1-Propanone, 1-[(3 β ,16 α ,17 β)-16-ethyl-3-(acetyloxy)androst-5-en-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

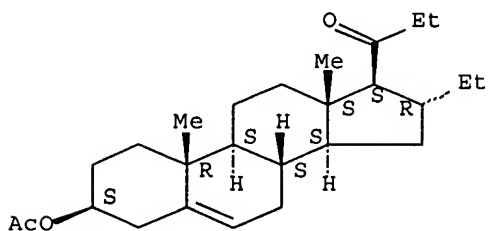


L11 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1967:517077 CAPLUS Full-text
 DOCUMENT NUMBER: 67:117077
 TITLE: 16 α -Alkyl-or 16 α -aryl-17 β -acyl
 derivatives of androstene
 INVENTOR(S): Maksimov, V. I.; Lur'i, F. A.; Morozova, L. S.
 PATENT ASSIGNEE(S): Ordzhonikidze, S., All-Union Scientific-Research
 Chemical-Pharmaceutical Institute
 SOURCE: U.S.S.R. From: Izobret., Prom. Obraztsy, Tovarnye
 Znaki 1966, 43(22), 37.
 CODEN: URXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Russian
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 188492		19661101	SU	19650701

GI For diagram(s), see printed CA Issue.
 AB The title compds. of the general formula I where the double bond is located between C-4 and C-5 or C-5 and C-6, R is O or H, β -OH, R1 is an alkyl or an aryl, are prepared by treating 17-cyanoandrost-5,16-dien-3-ol with excess alkylmagnesium halide in an organic solvent medium, e.g. anisole, at 60-85°, in a current of N. The resulting product is subjected to saponification and oxidation
 IT 16321-62-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 16321-62-3 CAPLUS
 CN 1-Propanone, 1-[(3 β ,16 α ,17 β)-16-ethyl-3-(acetyloxy)androst-5-en-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 3 OF 3 USPATFULL on STN

ACCESSION NUMBER: 2002:60938 USPATFULL Full-text
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
Hall, Andrea, New York, NY, UNITED STATES
Manga, Prashiela, New York, NY, UNITED STATES

APPLICANT

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-141563P	19990629 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	92	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	4216	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

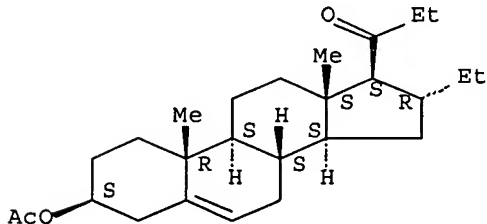
IT 16321-62-3

(methods and compns. that affect melanogenesis)

RN 16321-62-3 USPATFULL

CN 1-Propanone, 1-[(3 β ,16 α ,17 β)-16-ethyl-3-(acetyloxy)androst-5-en-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

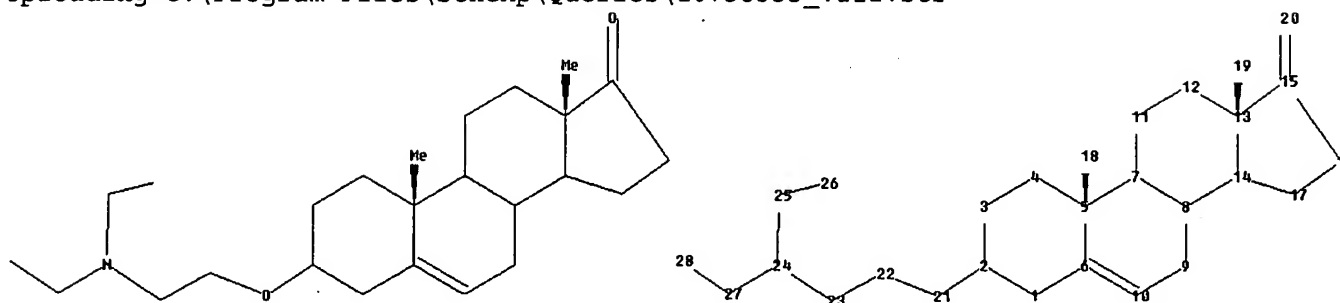


Compound VIII

=> file registry

=>

Uploading C:\Program Files\Stnexp\Queries\10758335_VIII.str



chain nodes :

18 19 20 21 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-21 5-18 13-19 15-20 21-22 22-23 23-24 24-25 24-27 25-26 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-21 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
12-13 13-14 13-15 14-17 15-16 15-20 16-17 21-22 23-24 24-25 24-27

exact bonds :

5-18 13-19 22-23 25-26 27-28

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

Stereo Bonds:

18-5 (Single Wedge).
19-13 (Single Wedge).

Stereo Chiral Centers:

5 (Parity=Even)
13 (Parity=Even)

Stereo RSS Sets:

Type=Relative (Default). 2 Nodes= 5 13
L12 STRUCTURE UPLOADED

=> d 112

L12 HAS NO ANSWERS

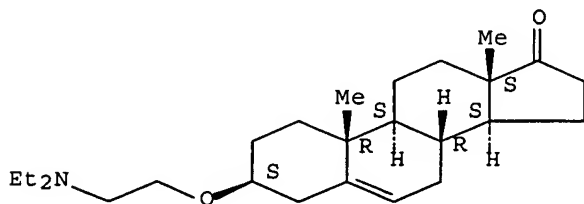
L12 STR

APPLICANT

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1383474	A2	20040128	EP 2002-776548	20020408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420
PRIORITY APPLN. INFO.:			US 1999-141563P	P 19990629
			US 2000-599487	A2 20000623
			US 2001-827428	A 20010406
			WO 2002-US11067	W 20020408
			US 2004-758335	A3 20040115
AB	The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.			
IT	2855-62-1 RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (methods and compns. that affect melanogenesis)			
RN	2855-62-1 CAPLUS			
CN	Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)			

Absolute stereochemistry.



TITLE: Species specificity of triphenylethylene derivatives and of compounds with a steroidal backbone for human and rat liver antiestrogen binding site (AEBS)

AUTHOR(S): van den Koedijk, C. D. M. A.; Govers, R. M. T.; Thijssen, J. H. H.; Blankenstein, M. A.

CORPORATE SOURCE: Fac. Pharm., Utrecht Univ., Utrecht, Neth.

SOURCE: Biochemical Pharmacology (1993), 46(10), 1870-2
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

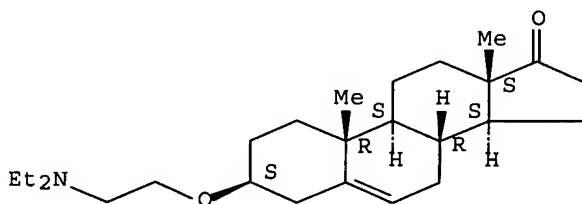
AB The binding affinity of derivs. of the triphenylethylene (TPE) antiestrogen tamoxifen and of steroidal compds. for human liver antiestrogen binding sites (AEBS) was compared with their binding affinity for rat liver AEBS. Despite the observation of some quant. differences overall a highly significant correlation between the relative binding affinity (RBA) for human and rat liver AEBS was found for all compds. tested ($r=0.93$, $N=19$). This was more pronounced for TPE derivs. ($r=0.83$, $N=12$) than for cholesterol derived compds. ($r=0.64$, $N=7$, not significant). The authors conclude that AEBS from rat liver can be used instead of human livers as a model to study the interactions of antiestrogens with AEBS.

IT 2855-62-1, LS3360
RL: BIOL (Biological study)
(antiestrogen-binding sites of liver of human and laboratory animal affinity for)

RN 2855-62-1 CAPLUS

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:504432 CAPLUS Full-text

DOCUMENT NUMBER: 117:104432

TITLE: Comparative affinity of steroidal and nonsteroidal antiestrogens, cholesterol derivatives and compounds with a dialkylamino side chain for the rat liver antiestrogen binding site

AUTHOR(S): Van den Koedijk, C. D. M. A.; Vis Van Heemst, C.; Elsendoorn, G. M.; Thijssen, J. H. H.; Blankenstein, M. A.

CORPORATE SOURCE: Dep. Pharm., Utrecht Univ., Utrecht, Neth.

SOURCE: Biochemical Pharmacology (1992), 43(12), 2511-18
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

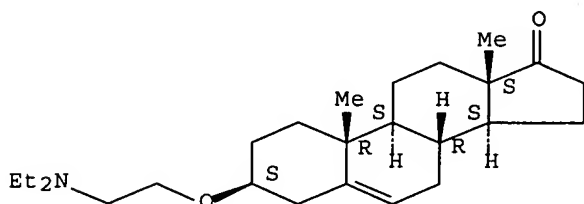
AB Steroidal and non-steroidal antiestrogens, steroidal compds. with (disubstituted) dialkyl amino side chain, cholesterol derivs., and histaminic and (anti)-progestational compds. were tested for their ability to compete with [3H]tamoxifen for the specific antiestrogen binding site (AEBS) in the post-mitochondrial fraction of rat liver homogenates. Relative binding affinity was highest for compds. with diethylamino or pyrrolidino ethoxy side chains. Affinity decreased with shortening of this side chain. No connection could be established between the carbon backbone of the compound and affinity, except for the presence of (sometimes aromatic) ring structures. Steroidal ring structures do not seem to be necessary for binding. The cholesterol derivs. showed very little affinity for the rat liver AEBS. Histamine, melatonin, and the (anti)-progestational compds. showed no affinity for the AEBS; evidently, the AEBS is not identical to receptors for these compds.

IT 2855-62-1, LS 3360
 RL: PRP (Properties)
 (antiestrogen binding site affinity of, mol. structure in relation to)

RN 2855-62-1 CAPLUS

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:179605 CAPLUS Full-text

DOCUMENT NUMBER: 104:179605

TITLE: The squalene-2,3-epoxide cyclase as a model for the development of new drugs

AUTHOR(S): Cattell, L.; Ceruti, M.; Viola, F.; Delprino, L.; Balliano, G.; Duriatti, A.; Bouvier-Nave, P.

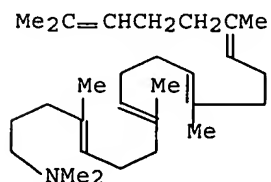
CORPORATE SOURCE: Ist. Chim. Farm. Appl., Univ. Torino, Turin, 10125, Italy

SOURCE: Lipids (1986), 21(1), 31-8
 CODEN: LPDSAP; ISSN: 0024-4201

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



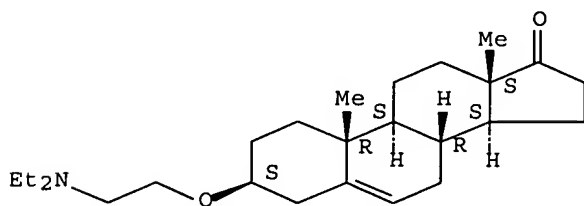
AB 2-Aza-2,3-dihydrosqualene (I) [86699-73-2] and its derivs. were tested as inhibitors of 2,3-oxidosqualene cyclase (EC 5.4.99.7) [9032-71-7]. Microsomes from different sources (germinated pea cotyledons, maize seedlings, rat liver, and yeasts) were used. The results indicate that I and its derivs. strongly inhibit the enzyme, the site of the enzyme responsible for binding to the inhibitor is quite sensitive to the steric hinderance, and the degree of the inhibitory activity is greater in higher plants than in rat liver or fungi.

IT 2855-62-1
RL: BIOL (Biological study)
(oxidosqualene cyclase inhibition by)

RN 2855-62-1 CAPLUS

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:91232 CAPLUS Full-text

DOCUMENT NUMBER: 62:91232

ORIGINAL REFERENCE NO.: 62:16336c-f

TITLE: Pharmacological 3 β -(aminomethoxy)-5-androsten-17-ones

PATENT ASSIGNEE(S): Upjohn Co.

SOURCE: 8 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NL 6404875		19641102	NL 1964-4875	19640501
PRIORITY APPLN. INFO.:			US	19630501

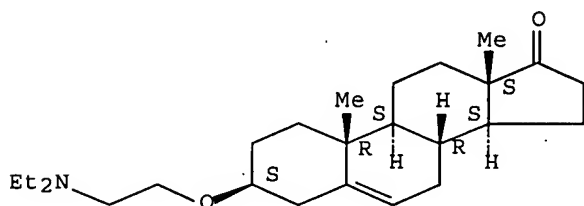
GI For diagram(s), see printed CA Issue.

AB I, in which R is NH₂, NEt₂, or NMeCH₂CH₂OH, are prepared by halogenating 3 β -(carboxymethoxy)-5-androsten-17-one (II), and then treating the formed 3 β -(haloformylmethoxy)-5-androsten-17-one with NH₃, NHet₂, or methylaminoethanol. Thus, 2 g. II is dissolved in 25 ml. tetrahydrofuran (THF) containing 3 drops pyridine and 5 ml. oxalyl chloride. The mixture is stirred 30 min. at 0°, then 30 min. at room temperature, the solution concentrated in vacuo <25°, and 25 ml. anhydrous C₆H₆ added. The solution is evaporated to dryness in vacuo, the obtained chloroformylmethoxy compound dissolved in 50 ml. THF, and 5 ml. NHet₂ added at 0°. The mixture is stirred 2 hrs. at room temperature, evaporated in vacuo, the residue dissolved in AcOEt, the solution washed successively with H₂O, dilute acid, dilute base and H₂O, and dried over

anhydrous sulfate. The organic solution is evaporated and recrystd. from a mixture of Skellysolve B hexanes and ether (3:2), and then recrystd. (ether) to yield 1.45 g. 3 β -(diethylcarbamoylmethoxy)-5-androstan-17-one (I, R = NEt₂) (Ia), m. 110-10.5°, [α]_D 5° (CHCl₃). Ia is useful as sedative and diuretic.

IT 2855-62-1P, Androst-5-en-17-one, 3 β -[2-(diethylamino)ethoxy]-
 RL: PREP (Preparation)
 (preparation of)
 RN 2855-62-1 CAPLUS
 CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:91231 CAPLUS Full-text

DOCUMENT NUMBER: 62:91231

ORIGINAL REFERENCE NO.: 62:16336a-c

TITLE: Steroid[3,2-b]pyridines

INVENTOR(S): Shimizu, Masao; Ota, Motokichi; Ueno, Katsujiro;
 Takegoshi, Toshio

PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 40003917	B4	19650302	JP	19620504

PRIORITY APPLN. INFO.: JP 19620504

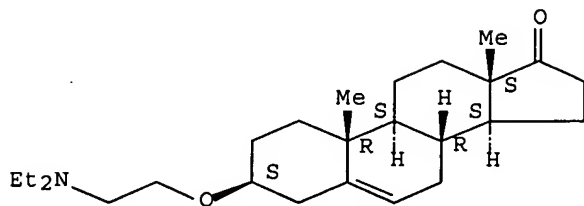
GI For diagram(s), see printed CA Issue.

AB A mixture of 4 g. 2-hydroxymethylene-17 β -hydroxyandrostan-3-one, 2 g. cyanoacetamide, 400 ml. EtOH, and 9.0 ml. NEt₃ is refluxed for 10 hrs., concentrated in vacuo, to the residue is added H₂O, and precipitated mass is recrystd. from MeOH (or AcOEt) to give I (R = CN, R' = O, R'' = H), m. >300°. Similarly are prepared the following I (R, R', R'', and m.p. given): CN, O, Me, >300°; CN, S, H, >300°; CN, S, Me, >300°. Also are prepared the following II (R, R', R'', and m.p. given): CONH₂, NH₂, Me, 250-2.5° (AcOEt); CONH₂, NH₂, H (having a double bond between 4-5), 274-6.5° (decomposition) (MeOH); CONH₂, NH₂, Me (having a double bond between 4-5), 196-7°/276-80° (double m.p.) (AcOEt); CO₂Et, NH₂, H, 140° (decomposition) (MeOH); CO₂Et, NH₂, Me (having a double bond between 4-5), 183-7° (MeOH).

IT 2855-62-1P, Androst-5-en-17-one, 3 β -[2-(diethylamino)ethoxy]-
 RL: PREP (Preparation)
 (preparation of)

RN 2855-62-1 CAPLUS
CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA
INDEX NAME)

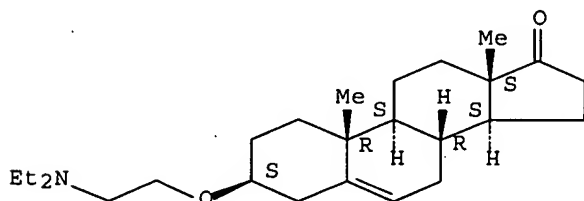
Absolute stereochemistry.



L14 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:461307 CAPLUS Full-text
DOCUMENT NUMBER: 59:61307
ORIGINAL REFERENCE NO.: 59:11197c
TITLE: 3 β - (Dialkylaminoalkoxy) -5-androstan-17-ones in
hypocholesterolemics
INVENTOR(S): Kagan, Fred
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: 9 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
FR M1721		19630408	FR	
PRIORITY APPLN. INFO.:			US	19610109
OTHER SOURCE(S):	MARPAT 59:61307			
AB	3 β - (Dialkylaminoalkoxy) -5-androsten-17-ones, 3 β - (dialkylaminoalkoxy)-5 α -androstan-17-ones, and their N-oxides are used in hypocholesterolemic compns. The dosage of the active ingredient is approx. 5-150 mg. 1-4 times a day.			
IT	2855-62-1, Androst-5-en-17-one, 3 β -[2-(diethylamino)ethoxy]- (in hypercholesterolemia treatment)			
RN	2855-62-1 CAPLUS			
CN	Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)			

Absolute stereochemistry.



L14 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:68617 CAPLUS Full-text

DOCUMENT NUMBER: 58:68617

ORIGINAL REFERENCE NO.: 58:11781f-h,11782a-b

TITLE: Cholesterol biosynthesis. V. The time course and pathway of the later stages of cholesterol biosynthesis in the livers of intact rats

AUTHOR(S): Goodman, DeWitt S.; Avigan, Joel; Steinberg, Daniel

CORPORATE SOURCE: U.S. Public Health Serv., Bethesda, MD

SOURCE: Journal of Biological Chemistry (1963), 238, 1287-93

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

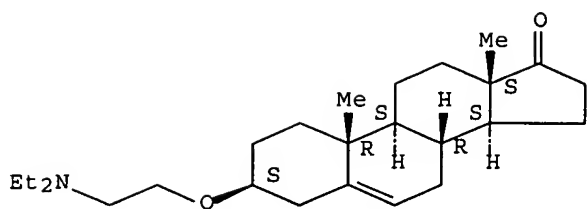
AB Studies have been conducted of the time course of the distribution of radioactivity in rat liver nonsaponifiables at several short intervals after the intravenous injection of 2-C¹⁴-DL-mevalonic acid. Recently developed thin-layer chromatographic techniques were employed that permit separation of many of the sterol intermediates in cholesterol biosynthesis. Both normal and triparanol-fed rats were studied, and biochem. techniques were used to aid in the identification of some of the intermediate compds. The appearance of radio-activity in liver sterol was extremely rapid. After 2 min. 7% of the injected radioactivity was present in liver nonsaponifiables, and 43% of this was contained in sterols; 57% of the nonsaponifiable radioactivity was present as squalene. After 30 min., 11% of the injected radioactivity was present in the nonsaponifiables, and 89% of this was contained in sterols. Within the sterol fraction, radioactivity was found primarily in lanosterol, an intermediate zone, Δ^7 (+ Δ^8)-cholestenol, and cholesterol. The relative amount of radioactivity in the first three of these decreased progressively from the maximum found at 2 min., which is consistent with the conclusion that these components lie on the major biosynthetic pathway to cholesterol. After 2 min., 53% of the sterol radioactivity was in lanosterol and only 19% in cholesterol; by 30 min., 76% of the sterol radioactivity was in cholesterol. The evidence presented suggests that the radioactivity in the intermediate zone from normal rats was contained in a C₂₈ sterol mixture containing compds. with both saturated and unsatd. side chains. The results also indicate that in normal rats no significant radioactivity was contained in $\Delta^7,24$ -cholestadienol or in zymosterol, whereas major amts. of radioactivity were present in one or both of these compds. in triparanol-treated rats. Only traces of radioactivity were found in 24,25-dihydrolanosterol and in desmosterol throughout the time period studied. It is probable that neither of these compds. lies on the major normal pathway of cholesterol biosynthesis. Reduction of the side chain probably occurs mainly at some intermediate stage in the sequence of reactions that modify the configuration of the sterol nucleus. Side chain reduction does not occur exclusively at any one point, however, but does occur to different degrees at several or perhaps at all points in the normal pathway from lanosterol to cholesterol.

IT 2855-62-1, Androst-5-en-17-one, 3 β -[2-(diethylamino)ethoxy]-
(in reduction of desmosterol and lanosterol)

RN 2855-62-1 CAPLUS

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:68616 CAPLUS Full-text

DOCUMENT NUMBER: 58:68616

ORIGINAL REFERENCE NO.: 58:11781e-f

TITLE: Cholesterol biosynthesis. IV. Reduction of lanosterol to 24,25-dihydrolanosterol by rat liver homogenates

AUTHOR(S): Avigan, Joel; Goodman, DeWitt S.; Steinberg, Daniel

CORPORATE SOURCE: U.S. Public Health Serv., Bethesda, MD

SOURCE: Journal of Biological Chemistry (1963), 238, 1283-6
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

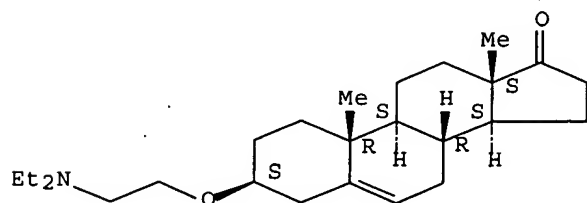
AB cf. CA 56, 10753i. The anaerobic reduction of labeled lanosterol, biosynthetically prepared from 2-C¹⁴-mevalonic acid, to 24,25-dihydrolanosterol has been demonstrated with rat liver homogenates. Enzymic activity was associated with cell particles, mostly with microsomes, and required reduced triphosphopyridine nucleotide. The enzyme was completely inhibited on addition of N-ethylmaleimide or p-chloromercuribenzoate, and did not require a bivalent cation for activity. Attempts to demonstrate the reversibility of side chain reduction of lanosterol during both anaerobic and aerobic incubations were not successful. Triparanol and two other inhibitors of cholesterol biosynthesis blocked the reduction of both lanosterol and desmosterol in vitro. Unlabeled lanosterol or desmosterol added to the incubation medium caused a comparable inhibition of reduction of C¹⁴-lanosterol. It is possible that a single enzyme is responsible for the reduction of both sterol substrates.

IT 2855-62-1, Androst-5-en-17-one, 3β-[2-(diethylamino)ethoxy] -
(in reduction of desmosterol and lanosterol)

RN 2855-62-1 CAPLUS

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3β)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 10 OF 10 USPATFULL on STN

ACCESSION NUMBER: 2002:60938 USPATFULL Full-text *APPLICANT*
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
Hall, Andrea, New York, NY, UNITED STATES
Manga, Prashiela, New York, NY, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-141563P	19990629 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	92	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	4216	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

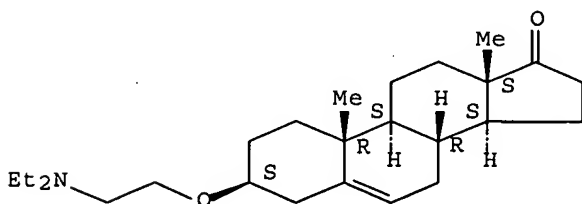
IT 2855-62-1

(methods and compns. that affect melanogenesis)

RN 2855-62-1 USPATFULL

CN Androst-5-en-17-one, 3-[2-(diethylamino)ethoxy]-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

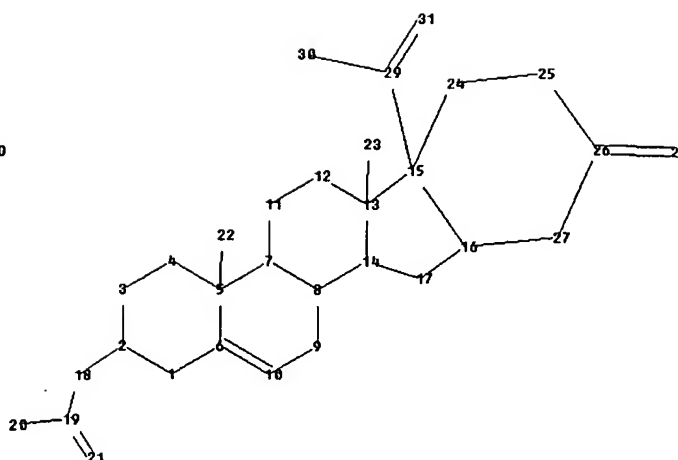
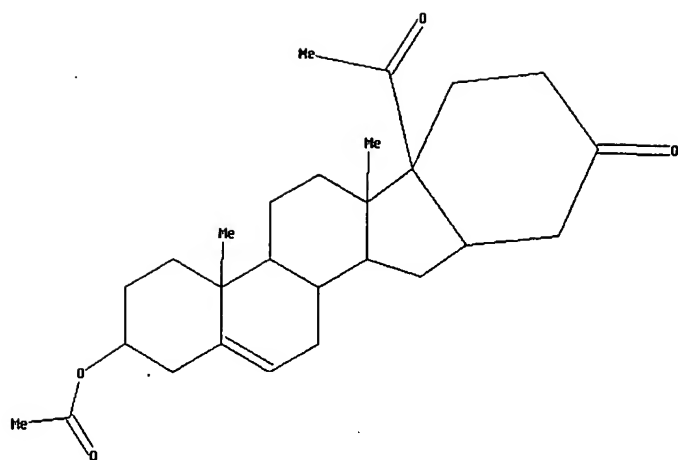


=> file registry

=>

Uploading C:\Program Files\Stnexp\Queries\10758335_II.str

Compound II



chain nodes :

18 19 20 21 22 23 28 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 24 25 26 27

chain bonds :

2-18 5-22 13-23 15-29 18-19 19-20 19-21 26-28 29-30 29-31

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13

13-14 13-15 14-17 15-16 15-24 16-17 16-27 24-25 25-26 26-27

exact/norm bonds :

1-2 1-6 2-3 2-18 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12

12-13 13-14 13-15 14-17 15-16 15-24 16-17 16-27 18-19 19-21 24-25 25-26

26-27 26-28

29-31

exact bonds :

5-22 13-23 15-29 19-20 29-30

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS

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22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS

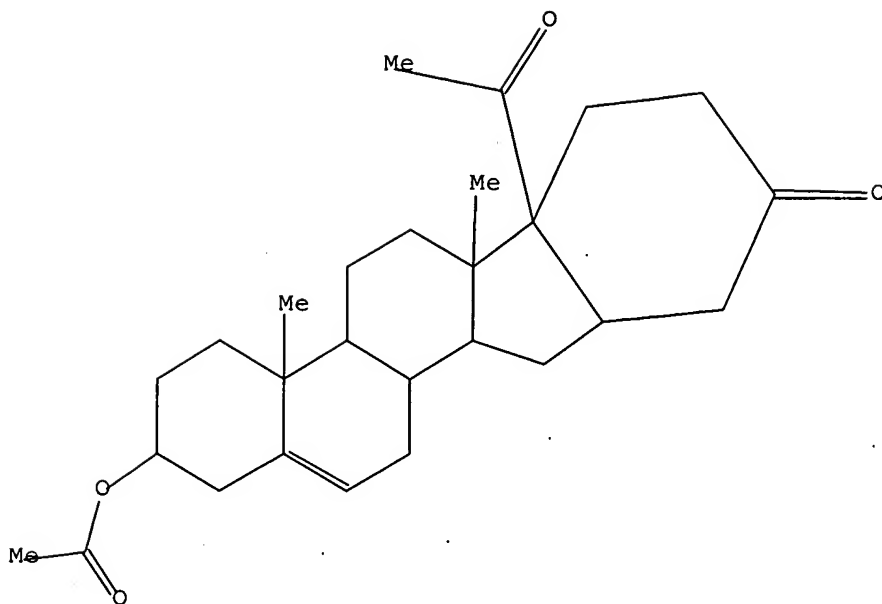
30:CLASS 31:CLASS

L15 STRUCTURE UPLOADED

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L15 HAS NO ANSWERS

L15 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 10:30:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 81 TO ITERATE

100.0% PROCESSED 81 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L16 1 SEA EXA FUL L15

=> file medline, caplus, wpids, uspatfull

=> s l16

SAMPLE SEARCH INITIATED 10:30:27 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 62
PROJECTED ANSWERS: 0 TO 0

L17 5 L16

=> d l17 1-5 ibib, abs, hitstr

L17 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:221159 CAPLUS Full-text
DOCUMENT NUMBER: 136:257280
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J.; Hall, Andrea; Manga, Prashiela

APPLICANT

PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U. S. Ser. No. 599,487.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1383474	A2	20040128	EP 2002-776548	20020408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420

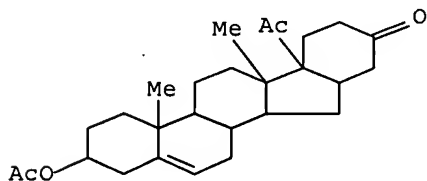
PRIORITY APPLN. INFO.:
 US 1999-141563P P 19990629
 US 2000-599487 A2 20000623
 US 2001-827428 A 20010406
 WO 2002-US11067 W 20020408
 US 2004-758335 A3 20040115

AB The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

IT 83117-73-1
 RL: COS (Cosmetic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (methods and compns. that affect melanogenesis)

RN 83117-73-1 CAPLUS

CN 16,24-Cyclo-21-norchol-5-en-23-one, 17-acetyl-3-(acetyloxy)-, (3 β ,16 β ,17 α)- (9CI) (CA INDEX NAME)



L17 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:162095 CAPLUS Full-text

DOCUMENT NUMBER: 104:162095

TITLE: Biological activity of transformed steroids. XXI.

Synthesis, conformational analysis and biological

activity of the D'7-pentarane, 16 α ,17 α -

cycloheptanoprogesterone

AUTHOR(S): Kamernitskii, A. V.; Levina, I. S.; Kulikova, L. E.;

Shamovskii, I. L.; Korkhov, V. V.; Nikitina, G. V.

CORPORATE SOURCE: Inst. Org. Khim., Moscow, USSR

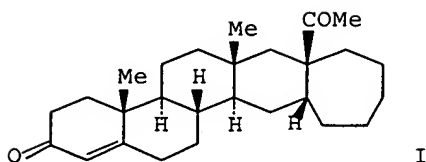
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1986), 20(1), 56-9

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



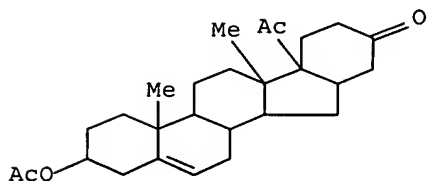
AB 16 α ,17 α -Cycloheptanoprogesterone (I) [101346-79-6] was synthesized; its conformation was described; and it was tested for progestogenic activity. I did not affect endometrium proliferation. This contrasted with the D'3-D'6-pentarane which did possess hormonal activity.

IT 83117-73-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)

RN 83117-73-1 CAPLUS

CN 16,24-Cyclo-21-norchol-5-en-23-one, 17-acetyl-3-(acetyloxy)-,
(3 β ,16 β ,17 α)- (9CI) (CA INDEX NAME)



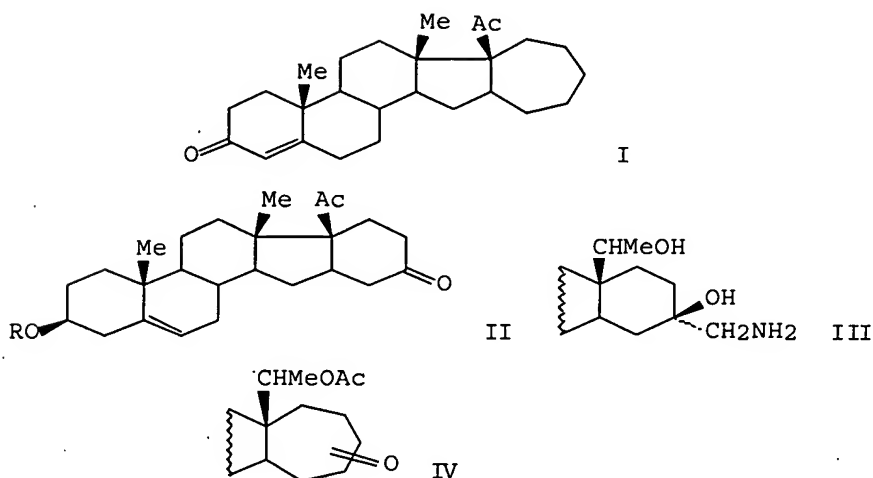
L17 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:179735 CAPLUS Full-text

DOCUMENT NUMBER: 98:179735

TITLE: Transformed steroids. 131. Ring D' homologation in
16 α ,17 α -cyclohexanopregnanes

AUTHOR(S): (D'6-pentaranes)
 Kamernitskii, A. V.; Kulikova, L. E.; Levina, I. S.
 CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya
 (1982), (11), 2552-7
 CODEN: IASKA6; ISSN: 0002-3353
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



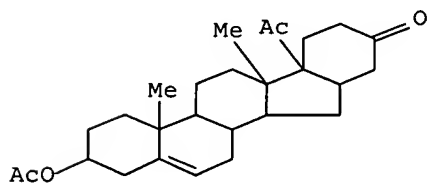
AB The cycloheptanopregnane I was prepared from the cyclohexanopregnene II (R = Ac) in 9 steps. Thus, II underwent successive cyanation, acetylation, and LiAlH_4 reduction to give the aminomethyl derivative III (R = H), which underwent Tiffeneau-Demjanov ring expansion and acetylation to give the cycloheptanopregnene IV. LiAlH_4 reduction of the tosylhydrazone of IV and subsequent Jones oxidation gave I. Ring expansion of II via addition reactions of CH_2N_2 or CH_2Br_2 were not successful.

IT 83117-73-1

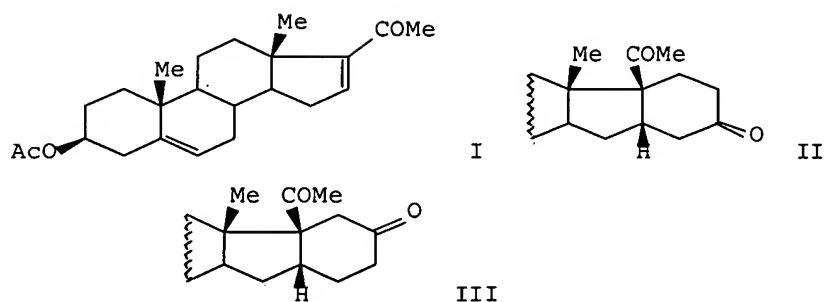
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of)

RN 83117-73-1 CAPLUS

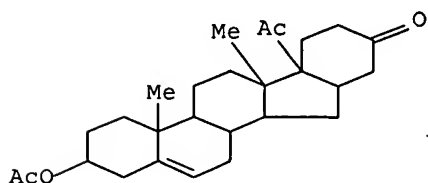
CN 16,24-Cyclo-21-norchol-5-en-23-one, 17-acetyl-3-(acetyloxy)-,
 (3 β ,16 β ,17 α)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1982:563316 CAPLUS Full-text
 DOCUMENT NUMBER: 97:163316
 TITLE: Transformed steroids. 125. Single-stage synthesis of
 oxo 16 α ,17 α -cyclohexanopregnanes under
 atmospheric and high pressure
 AUTHOR(S): Levina, I. S.; Kulikova, L. E.; El'yanov, B. S.
 CORPORATE SOURCE: Inst. Org. Khim., Moscow, USSR
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya
 (1982), (6), 1399-401
 CODEN: IASKA6; ISSN: 0002-3353
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB Cycloaddn. of the dehydropregnenolone acetate I with $\text{H}_2\text{C}:\text{C}(\text{OSiMe}_3)\text{CH}:\text{CH}_2$ in CH_2Cl_2 at 80° and 14 kbar gave a mixture of regioisomeric ketones II and III. Similar cyclization of I in the presence of AlCl_3 gave only II.
 IT 83117-73-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis-oxidation of)
 RN 83117-73-1 CAPLUS
 CN 16,24-Cyclo-21-norchol-5-en-23-one, 17-acetyl-3-(acetyloxy)-,
 (3 β ,16 β ,17 α)- (9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 5 USPATFULL on STN

ACCESSION NUMBER: 2002:60938 USPATFULL Full-text
 TITLE: Methods and compositions that affect melanogenesis
 INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
 Hall, Andrea, New York, NY, UNITED STATES
 Manga, Prashiela, New York, NY, UNITED STATES

APPLICANT

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-141563P	19990629 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	92	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	4216	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

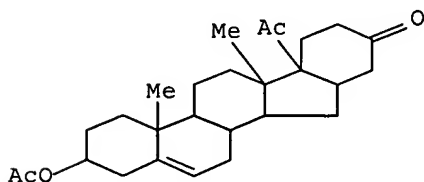
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 83117-73-1

(methods and compns. that affect melanogenesis)

RN 83117-73-1 USPATFULL

CN 16,24-Cyclo-21-norchol-5-en-23-one, 17-acetyl-3-(acetyloxy)-, (3 β ,16 β ,17 α)- (9CI) (CA INDEX NAME)

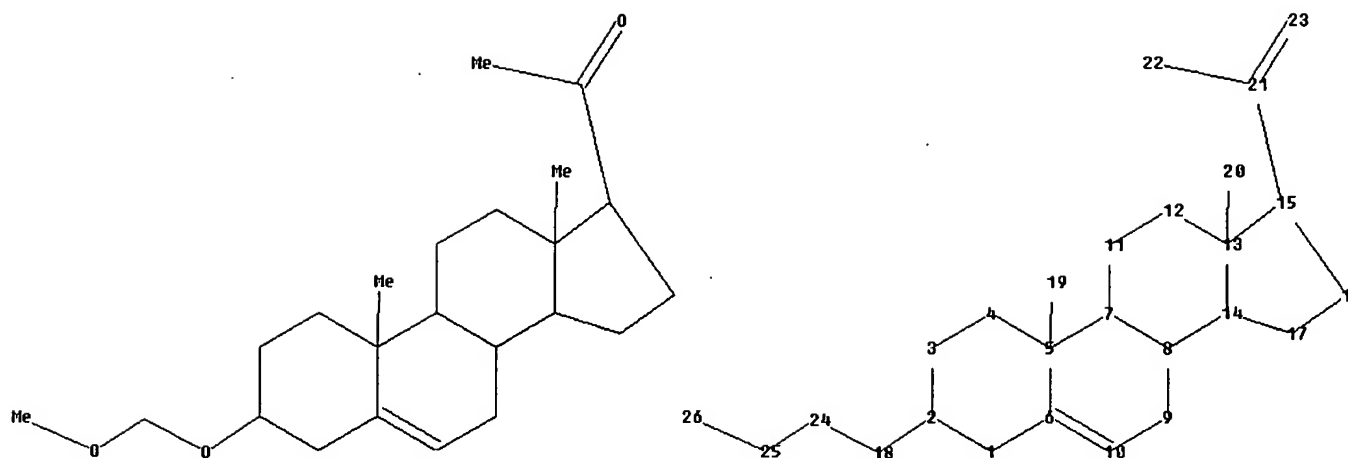


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Compound IV



chain nodes :

18 19 20 21 22 23 24 25 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-18 5-19 13-20 15-21 18-24 21-22 21-23 24-25 25-26

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-18 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
12-13 13-14 13-15 14-17 15-16 16-17 18-24 21-23 24-25

exact bonds :

5-19 13-20 15-21 21-22 25-26

Match level :

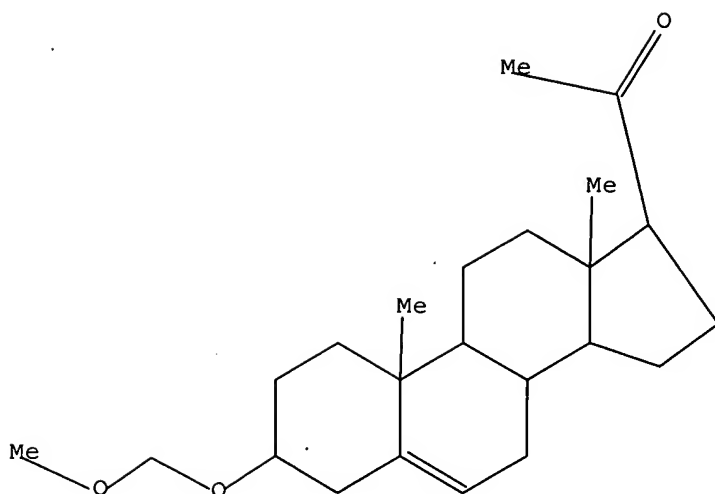
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L18 STRUCTURE UPLOADED

=> d 118

L18 HAS NO ANSWERS

L18 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l18 exa full

FULL SEARCH INITIATED 10:32:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L19 1 SEA EXA FUL L18

=> file medline, caplus, wpids, uspatfull

=> s l19

SAMPLE SEARCH INITIATED 10:32:28 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1 TO 40
PROJECTED ANSWERS: 0 TO 0

L20 17 L19

=> s l20 not py>2001

L21 13 L20 NOT PY>2001

=> d l21 1-13 ibib, abs, hitstr

L21 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:743150 CAPLUS Full-text
DOCUMENT NUMBER: 134:29610
TITLE: Highly β -selective epoxidation of
 Δ^5 -unsaturated steroids catalyzed by ketones

AUTHOR(S): Yang, Dan; Jiao, Guan-Sheng
CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong,
Hong Kong, Peop. Rep. China
SOURCE: Chemistry--A European Journal (2000), 6(19), 3517-3521
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:29610

AB A general catalytic and environmentally friendly method for β -epoxidn. of Δ^5 -unsatd. steroids has been developed, which uses ketones as the catalysts and Oxone as the terminal oxidant. A whole range of Δ^5 -unsatd. steroids, which bear different functional groups such as hydroxyl, carbonyl, acetyl, or ketal, as well as different side chains, were conveniently converted to the corresponding synthetically and biol. interesting $5\beta,5\beta$ -epoxides with excellent β -selectivities and high yields.

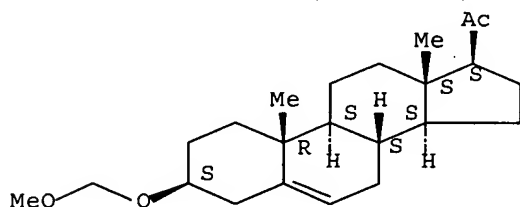
IT 23328-05-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(highly β -selective epoxidn. of Δ^5 -unsatd. steroids
catalyzed by ketones)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:424324 CAPLUS Full-text

DOCUMENT NUMBER: 113:24324

TITLE: Steroids. Part CCCXLVII. Synthesis and in vitro
antimetabolic evaluation of some steroidal thiazoles

AUTHOR(S): Drasar, Pavel; Pouzar, Vladimir; Cerny, Ivan; Pettit,
George R.; Havel, Miroslav

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague,
166 10, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications
(1989), 54(12), 3339-47

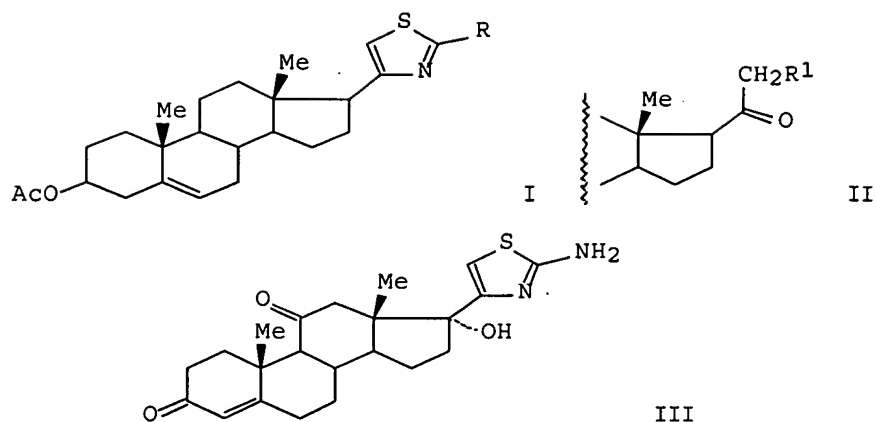
CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:24324

GI



AB Steroidal thiazoles I (R = NH₂, NHMe, NHPh, NMe₂, Ph, Me, CH₂CO₂Me) have been synthesized. The starting bromo ketone II (R¹ = Br) was prepared by bromination of pregnen-20-ones II (R¹ = H) with copper (II) bromide, and was used for synthesis of the thiazole derivs. employing the Hantzsch reaction. Preliminary biol. evaluation of thiazoles I and III against the P388 lymphocytic leukemia cell showed growth inhibition values of ED₅₀ 2.9 and 7 µg/mL for thiazoles III and I (R = NH₂), resp. Other I were less active.

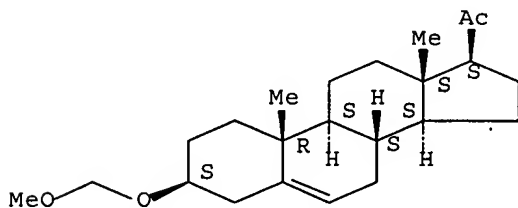
IT 23328-05-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of, with cupric bromide)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:477151 CAPLUS Full-text

DOCUMENT NUMBER: 111:77151

TITLE: Determination of the absolute configuration of secondary alcohols by modified Horeau's method using HPLC

AUTHOR(S): Svatos, Ales; Valterova, Irena; Fabryova, Anna; Vrkoc, Jan

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1989), 54(1), 151-9

CODEN: CCCCAC; ISSN: 0010-0765

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:77151

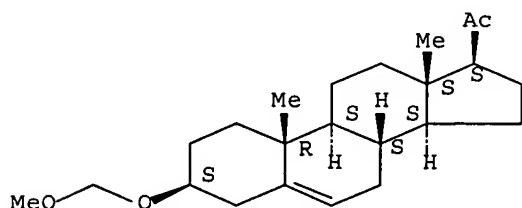
AB A method for determination of absolute configuration of secondary alcs., based on a modified Horeau's method, has been developed. The ratio of (1R,2'S)- and (1R,2'R)-N-[1-(1-naphthyl)ethyl]-2-phenylbutanamides was determined by HPLC on a straight phase. The method was tested on a series of steroid and terpene model compds. and was used in the determination of absolute configuration of 15-ripperten-3 α -ol, the defense substance of *Nasutitermes nigriceps* termites. The sensitivity of the determination is 100 nmol of the alc.

IT 23328-05-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:473791 CAPLUS Full-text

DOCUMENT NUMBER: 109:73791

TITLE: Steroids. CCCXXXIII. β -Glucosides of steroidal unsaturated nitriles

AUTHOR(S): Cerny, Ivan; Pouzar, Vladimir; Drasar, Pavel; Havel, Miroslav

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1987), 52(10), 2521-33

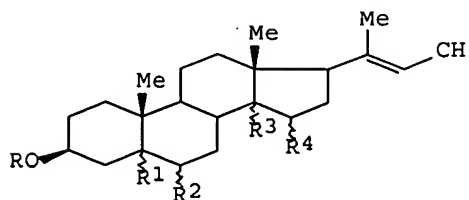
CODEN: CCCCAC; ISSN: 0366-547X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:73791

GI



I

AB Glycosides I (R = β -D-glucopyranosyl; R1 = α -H, β -H, R2-R4 = H; R1R2 = bond, R3R4 = bond, H2) were obtained by treating pregnan-2-ones with NCCH₂P(O)(OEt)₂ followed by deblocking and glycosidation. I (R = COCH₂CH₂CO₂H) were similarly prepared I (R = β -D-glucopyranosyl, R1R2 = bond, R3 = R4 = H) was also prepared by glycosidation of 3 β -hydroxy-5-pregnen-20-one; followed by reaction with NCCH₂P(O)(OEt)₂.

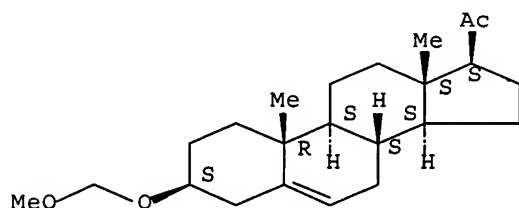
IT 23328-05-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanomethylphosphonate)

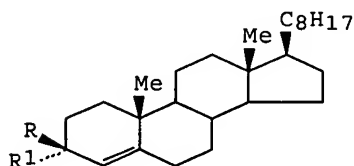
RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1987:554591 CAPLUS Full-text
 DOCUMENT NUMBER: 107:154591
 TITLE: Dehydrogenation of cyanamides. An approach to cyanimides and carbonyl compounds
 AUTHOR(S): Carrau, Reyes; Freire, Raimundo; Hernandez, Rosendo; Suarez, Ernesto
 CORPORATE SOURCE: Inst. Prod. Nat. Org., CSIC, La Laguna, Spain
 SOURCE: Synthesis (1986), (12), 1055-8
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:154591
 GI



AB Treatment of cyanamides with Pb(OAc)₄ afforded the corresponding cyanimides in high yields. Thus, cholestene I (R = NHCN, R1 = H) was treated with Ph (OAc)

in cyclohexane to give 87%, I (RR1 = NCN). These compds. were hydrolyzed to carbonyl compds. This sequence of reactions allows the synthesis of aldehydes and ketones from primary amines.

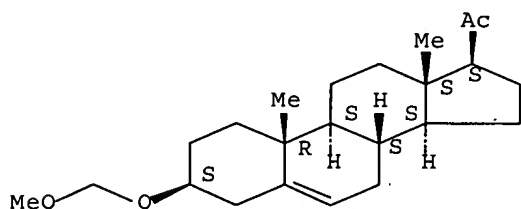
IT 23328-05-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:18930 CAPLUS Full-text

DOCUMENT NUMBER: 106:18930

TITLE: Infrared spectra of compounds with a methoxymethyl protecting group

AUTHOR(S): Vasickova, Sona; Pouzar, Vladimir; Cerny, Ivan; Drasar, Pavel; Havel, Miroslav

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10/6, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1986), 51(1), 90-100

CODEN: CCCCAK; ISSN: 0366-547X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:18930

AB IR spectra of a series of methoxymethyl steroidal ethers were studied. All the spectra exhibit three characteristic strong absorption bands due to coupled stretching vibrations of the C-O-C-O-C grouping in the region 1200-1000 cm⁻¹.

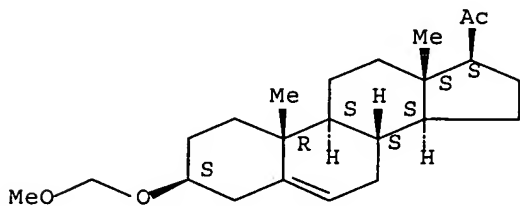
IT 23328-05-4

RL: PRP (Properties)
(IR spectrum of)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1987:18927 CAPLUS Full-text

DOCUMENT NUMBER: 106:18927

TITLE: Steroids. CCCXVIII. Steroids with the
 β -crotonate (2-butenate) side chain

AUTHOR(S): Cerny, Ivan; Pouzar, Vladimir; Drasar, Pavel; Turecek,
 Frantisek; Havel, Miroslav

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague,
 166 10/6, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications
 (1986), 51(1), 128-40

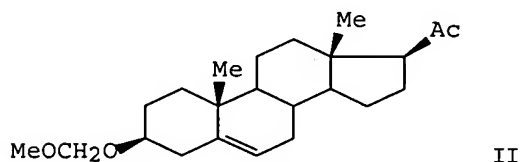
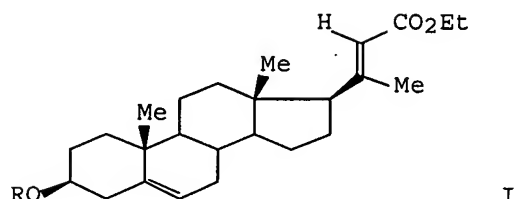
CODEN: CCCCAK; ISSN: 0366-547X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:18927

GI



AB 24-Nor-5,20(22)-choladienoate I (R = CH₂OMe) was prepared by the Wittig-Horner reaction of ketone II with di-Et ethoxycarbonylmethylphosphonate. The reaction afforded exclusively the E isomer. The structure of I (R = CH₂OMe) was confirmed by proton and carbon-13 NMR spectroscopy. I (R = CH₂OMe) was further converted into the 3-O-succinyl derivative I (R = COCH₂CH₂CO₂H). The 5 α ,6- and 5 β ,6-dihydro and Δ 5,14 analogs of I were also prepared and they were converted into their corresponding 3-O-succinyl derivs.

IT 23328-05-4

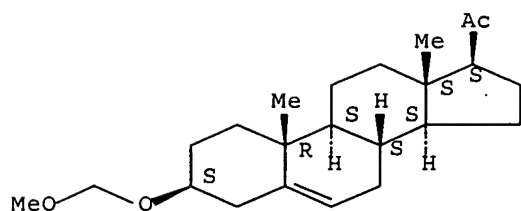
RL: RCT (Reactant); RACT (Reactant or reagent)

(Peterson olefination and Wittig-Horner reaction of)

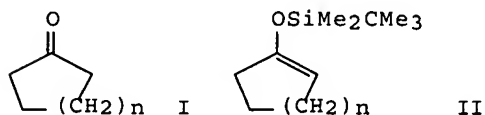
RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1985:204013 CAPLUS Full-text
 DOCUMENT NUMBER: 102:204013
 TITLE: Synthesis of tert-butyldimethylsilyl enol ethers from sterically hindered ketones
 AUTHOR(S): Mander, Lewis N.; Sethi, S. Paul
 CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
 SOURCE: Tetrahedron Letters (1984), 25(51), 5953-6
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Ketones, e.g., (I), react rapidly with t-butyldimethylsilyl triflate and amine bases to form t-butyldimethylsilyl enol ethers, e.g., II, in 90-100% yields.

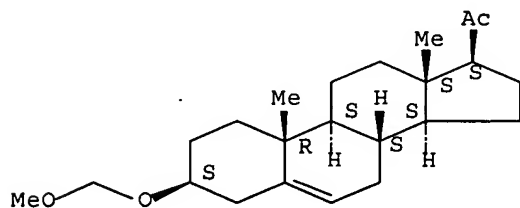
IT 23328-05-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation of, with tert-butyldimethylsilyl triflate)

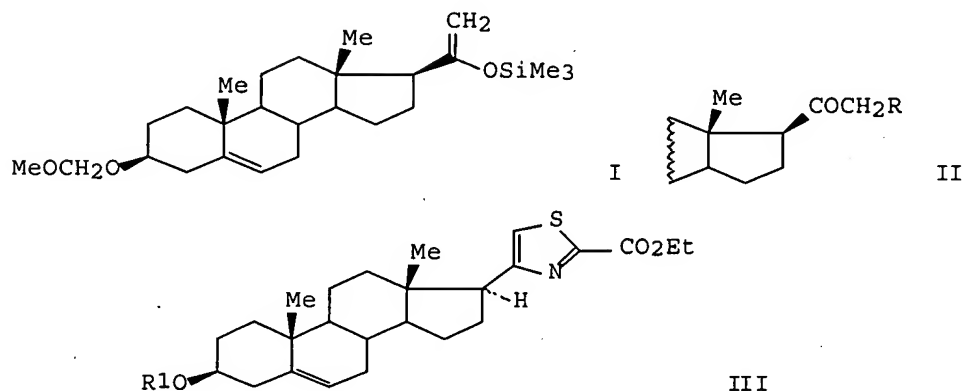
RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1984:571591 CAPLUS Full-text
 DOCUMENT NUMBER: 101:171591
 TITLE: Steroids. Part CCCVII. Synthesis of
 17 β -[4-(1,3-thiazoyl)]androstane
 3 β -hemisuccinate and glycoside
 AUTHOR(S): Drasar, Pavel; Pouzar, Vladimir; Cerny, Ivan;
 Smolikova, Jorga; Havel, Miroslav
 CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague,
 166 10/6, Czech.
 SOURCE: Collection of Czechoslovak Chemical Communications
 (1984), 49(4), 1039-50
 CODEN: CCCCAK; ISSN: 0366-547X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The pregnenone enol silyl ether I was oxidized by N-methylmorpholine
 oxide/OsO₄ to give the hydroxy ketone II (R = OH), which underwent mesylation
 and bromination to give II (R = Br). Hantzsch reaction of the latter with
 EtO₂CD(S)NH₂ gave the androstanylthiazole III (R₁ = H), which was converted to
 III (R₁ = HO₂CCH₂CH₂CO; β -D-glucopyranosyl).

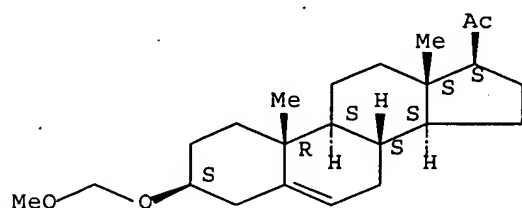
IT 23328-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and enolization-silylation of)

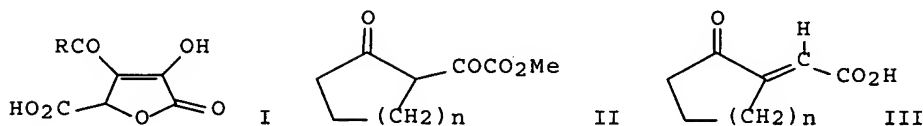
RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1984:191667 CAPLUS Full-text
 DOCUMENT NUMBER: 100:191667
 TITLE: Condensation of α,γ -diketo (or ketosuccinic) esters with glyoxylic acid
 AUTHOR(S): Bonadies, Francesco; Scarpati, Maria Luisa
 CORPORATE SOURCE: Ist. Chim. Org., Univ. Roma "La Sapienza", Rome, I-00185, Italy
 SOURCE: Gazzetta Chimica Italiana (1983), 113(7-8), 421-5
 CODEN: GCITA9; ISSN: 0016-5603
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 100:191667
 GI



AB Cyclocondensation of $\text{RCOCH:C(OH)CO}_2\text{Me}$ [$\text{R} = \text{Me}, \text{Me}_2\text{CH}, \text{Me}_2\text{CHCH}_2, \text{Ph. OEt}, 3\beta\text{-(methoxymethoxy)androst-5-en-17}\beta\text{-yl}$] with NaO_2CCHO gave butenolides I, which underwent elimination reaction in the presence of Zn(OAc)_2 to give $\text{RCOCH}_2\text{CH(OH)CO}_2\text{H}$ in 45-87% yields. Condensation of β -substituted dioxo esters, i.e. cycloalkanones II ($n = 1, 2$), with NaO_2CCHO gave α,β -unsatd. acids, i.e. acrylic acids III.

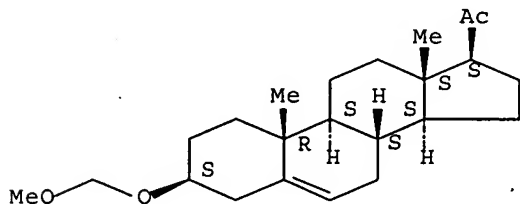
IT 23328-05-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and condensation of, with di-Me oxalate)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



TITLE: Alkyl-, aryl-, vinyl-, and heterosubstituted organozirconium compounds - selective nucleophiles of low basicity

AUTHOR(S): Weidmann, Beat; Maycock, Christopher D.; Seebach, Dieter

CORPORATE SOURCE: Lab. Org. Chem., Swiss Fed. Inst. Technol., Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1981), 64(5), 1552-7
CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:5735

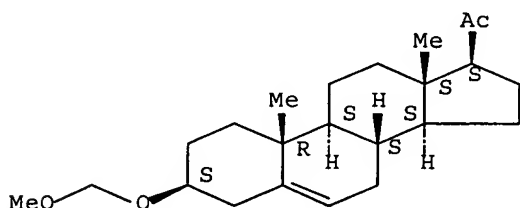
AB Solns. of the title compds. are accessible from organolithium reagents and trialkoxyzirconium chloride. In contrast to their Ti analogs, vinylzirconium reagents are stable enough to be employed. Generally, organozirconium reagents are highly selective carbonylphiles of exceedingly low basicity for aldehydes and ketones.

IT 23328-05-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with organozirconium compds.)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:435622 CAPLUS Full-text

DOCUMENT NUMBER: 73:35622

TITLE: Steroids and related natural products. XLVIII.
Bufadienolides. 1. Introduction and base-catalyzed condensation of methyl ketones with glyoxylic acid

AUTHOR(S): Pettit, George R.; Green, Brian; Dunn, George L.

CORPORATE SOURCE: Dep. of Chem., Arizona State Univ., Tempe, AZ, USA

SOURCE: Journal of Organic Chemistry (1970), 35(5), 1367-76
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A comprehensive study of an aldol condensation between glyoxylic acid and various Me ketones was described. At high hydroxyl ion concentration, methyl β -naphthyl ketone gave bis(β -naphthacyl)acetic acid but by careful control of pH the condensation could be directed to yield trans- β -naphthoyleacrylic acid and (or) a mixture of α -hydroxy- γ -oxobutyric acid and α -methoxy- γ -oxobutyric acid. The reaction was applied to Me cyclopentyl ketone, 2,5-dimethoxyacetophenone, 2,4-dimethylacetophenone, pinonic acid, and the steroidal ketones, 3 β -hydroxy-20-oxo-5-pregnene and 3 β -hydroxy-20-oxo-5 α -pregnane.

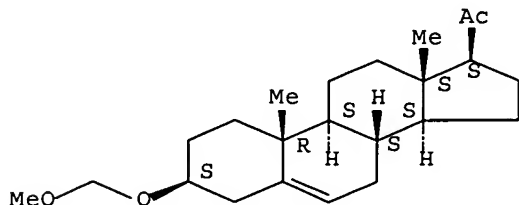
IT 23328-05-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23328-05-4 CAPLUS

CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:53631 CAPLUS Full-text
DOCUMENT NUMBER: 58:53631
ORIGINAL REFERENCE NO.: 58:9193f-h,9194a-c
TITLE: Lower alkoxy)methyl ether derivatives of steroids
INVENTOR(S): Fried, Josef
PATENT ASSIGNEE(S): Olin Mathieson Chemical Corp.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3062846	---	19621106	US 1961-106178	19610428
PRIORITY APPLN. INFO.:			US	19610428
OTHER SOURCE(S):	CASREACT 58:53631			

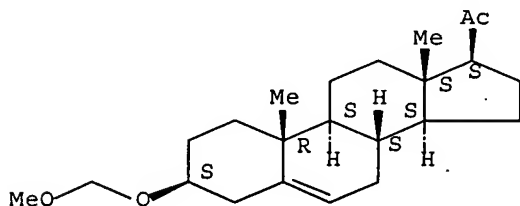
GI For diagram(s), see printed CA Issue.

AB The preparation was described of a (lower alkoxy)methyl ether derivative of a steroid having an unhindered primary or secondary OH group by treating said steroid with a lower alkyl acetal of HCHO and HCHO (or a source of HCHO) in the presence of a strong-acid catalyst. By unhindered steroids was meant steroids containing an OH group at 1 or more of the following positions: 1 α , 1 β , 2 α , 2 β , 3 α , 3 β , 4 α , 4 β , 6 α , 6 β , 7 α , 7 β , 11 α , 12 α , 12 β , 15 α , 15 β , 16 α , 16 β , 18, or 19; such steroids included those of the androstane series containing a 17 α - or 17 β -OH group and those of the pregnane series containing a 20 α -, 20 β -, or 21-OH group. The preferred steroids were those of the pregnane series, particularly those of the general formula I, wherein positions 1,2; 4,5; 5,6; and 6,7 are saturated or double-bonded, R is H, R is α -OH, α -acyl-oxy, β -OH, or β -acyloxy, or together R and R' is oxo, R is H, R''' is α -OH, α -acyloxy, or β -OH, or together R'' and R''' is oxo, the 2 X are the same or different and represent H, halo, or lower alkyl, at least 1 X being H, Y is H, OH, or acyloxy, Y' is H or Me, Y'' is H, halo, or Me, Z is H or OH, and Z' is H, halo, OH, acyloxy, or Me. (Ultraviolet spectra in EtOH; infrared spectra in Nujol mulls; $[\alpha]_D$ in CHCl₃). To 1 g. 3 β -hydroxypregn-5-en-20-one (Ia) suspended in 50 ml. CH₂(OMe)₂ (II) and 20 g. trioxane (III) was added 0.5 ml. 70% HClO₄ with stirring, the resulting solution kept 20 min., treated with 6 m°. N NaOH, diluted with H₂O, the II and III removed in vacuo, and the

product in the residual suspension isolated with CHCl_3 to give 1.18 g. 3-methoxymethyl ether derivative of Ia, m. 102-4° (Me₂CO-hexane), $[\alpha]_D^{19}$ (c 1.32), γ 5.87 and 6.02. μ . The following addnl. compds. were prepared [compound, m.p., $[\alpha]_{23D}$, 11 α (ϵ) γ (μ) given]: 11-methoxymethyl ether deriv, of 11 α -hydroxyprogesterone, 138-9° (Me₂CO-hexane), 169° (c 1.37), 241 (16,000), 5.91, 6.02, and 6.22; 21-methoxymethyl ether derivative of 9 α -fluoro-17-hydroxycorticosterone, 288-94°, 43° (c 0.65), 238 (15,700), 2.91, 5.82, 6.0, and 6.15 (shoulder); 16 α ,21-bis(methoxymethyl) ether derivative of triamcinolone (IV), 218-19° (95% EtOH), 34° (c 1.1), --, 2.92, 5.81, 6.0, 6.14, 6.22; 16 α -methoxymethyl ether derivative (V) of IV, 220-3°, 42° (c 0.52), --, 2.95, 5.88, 6.02, 6.18, 6.23 [V 21-acetate m. 178-80° (Me₂CO-hexane), $[\alpha]_{23D}$ 32° (c 1.02), λ 239 m μ (ϵ 16,500), λ 2.92, 5.71, 5.79, 6.01, 6.18, 6.23 μ]; 16,21-bis(methoxymethyl) ether derivative of 9 α -fluoro-16 α -hydroxyprednisone, 139-40°, 83° (c 0.41), 234 (14,000), 3.03, 5.80, 6.01, 6.17, 6.23; 16,21-bis(methoxymethyl) ether derivative of 16 α ,17 α -dihydroxy-9 α -fluorocorticosterone, 2130° 70° (c 0.43), 239 (15,500), 2.92, 5.84, 5.99, 6.15. The alkoxymethyl ether derivs. are used as intermediates, and those compds. which are alkoxymethyl ether derivs. of physiol. active steroids retain their activity and hence can be used for the same purpose as the parent compound

IT 23328-05-4P, Pregn-5-en-20-one, 3 β -(methoxymethoxy) -
 RL: PREP (Preparation)
 (preparation of)
 RN 23328-05-4 CAPLUS
 CN Pregn-5-en-20-one, 3-(methoxymethoxy)-, (3 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 10:17:43 ON 08 JAN 2007)

FILE 'REGISTRY' ENTERED AT 10:17:54 ON 08 JAN 2007

L1 STRUCTURE UPLOADED
 L2 0 S L1
 L3 1 S L1 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:18:50 ON 08 JAN 2007

L4 9 S L3

FILE 'REGISTRY' ENTERED AT 10:20:25 ON 08 JAN 2007

L5 STRUCTURE UPLOADED
 L6 0 S L5
 L7 1 S L5 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:21:21 ON 08 JAN 2007

L8 8 S L7

FILE 'REGISTRY' ENTERED AT 10:22:43 ON 08 JAN 2007

L9 STRUCTURE UPLOADED

L10 1 S L9 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:23:15 ON 08 JAN 2007

L11 3 S L10

FILE 'REGISTRY' ENTERED AT 10:26:09 ON 08 JAN 2007

L12 STRUCTURE UPLOADED

L13 2 S L12 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:26:46 ON 08 JAN 2007

L14 10 S L13

FILE 'REGISTRY' ENTERED AT 10:29:49 ON 08 JAN 2007

L15 STRUCTURE UPLOADED

L16 1 S L15 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:30:21 ON 08 JAN 2007

L17 5 S L16

FILE 'REGISTRY' ENTERED AT 10:31:52 ON 08 JAN 2007

L18 STRUCTURE UPLOADED

L19 1 S L18 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:32:23 ON 08 JAN 2007

L20 17 S L19

L21 13 S L20 NOT PY>2001

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

77.45

657.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-10.14

-32.76

STN INTERNATIONAL LOGOFF AT 10:33:21 ON 08 JAN 2007

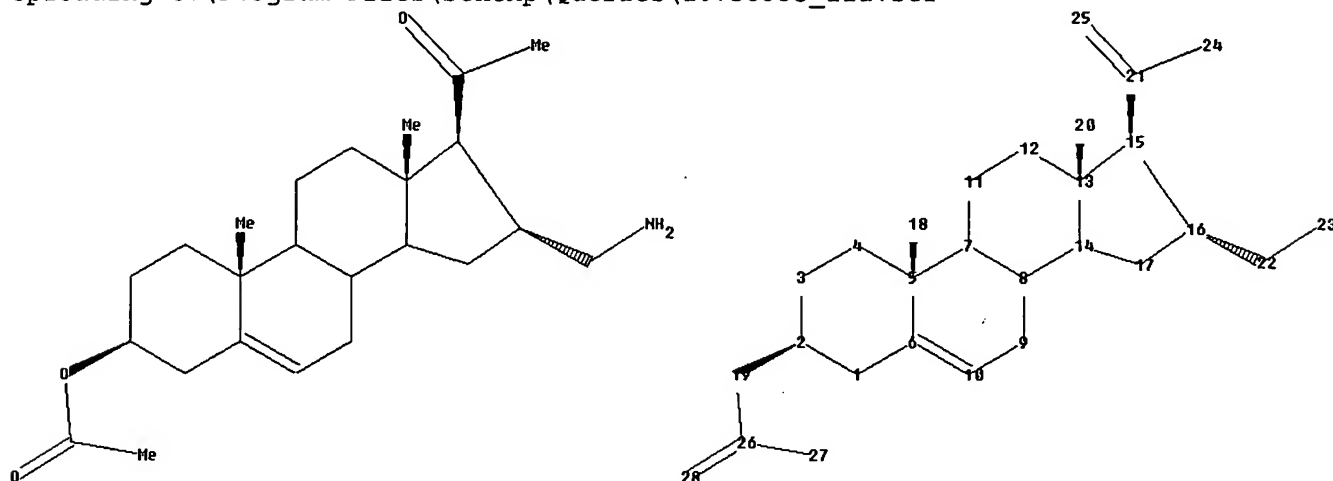
FILE 'HOME' ENTERED AT 10:13:11 ON 08 JAN 2007

Compound III

=> file registry

=>

Uploading C:\Program Files\Stnexp\Queries\10758335_III.str



chain nodes :

18 19 20 21 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-19 5-18 13-20 15-21 16-22 19-26 21-24 21-25 22-23 26-27 26-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 13-15 14-17 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12
12-13 13-14 13-15 14-17 15-16 16-17 19-26 21-25 22-23 26-28

exact bonds :

5-18 13-20 15-21 16-22 21-24 26-27

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

Stereo Bonds:

18-5 (Single Wedge).
19-2 (Single Wedge).
20-13 (Single Wedge).
21-15 (Single Wedge).
22-16 (Single Hash).

Stereo Chiral Centers:

2 (Parity=Odd)
5 (Parity=Even)
13 (Parity=Even)
15 (Parity=Odd)

16 (Parity=Even)

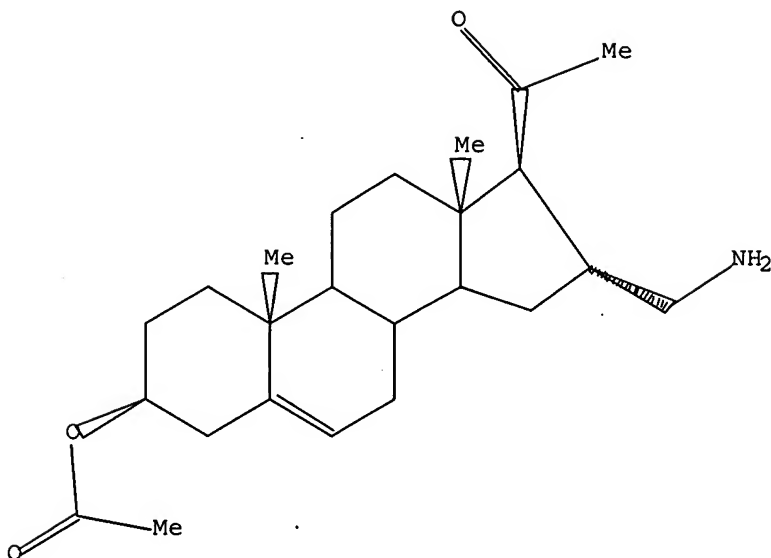
Stereo RSS Sets:

Type=Relative (Default). 5 Nodes= 2 5 13 15 16
L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:13:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9 TO 360

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 exa full

FULL SEARCH INITIATED 10:13:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS

1 ANSWERS

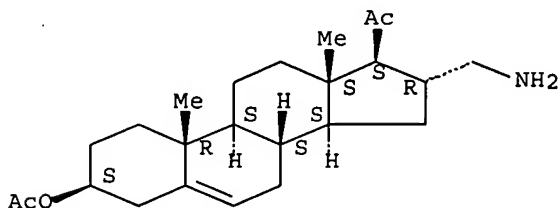
SEARCH TIME: 00.00.01

L3 1 SEA EXA FUL L1

=> d 13

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 404886-31-3 REGISTRY
ED Entered STN: 10 Apr 2002
CN Pregn-5-en-20-one, 3-(acetyloxy)-16-(aminomethyl)-, (3 β ,16 α)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
DR 23738-13-8
MF C24 H37 N O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file medline, caplus, wpids, uspatfull

=> s 13

SAMPLE SEARCH INITIATED 10:14:19 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L4 3 L3

=> d 14 1-3 ibib, abs

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:221159 CAPLUS Full-text
DOCUMENT NUMBER: 136:257280
TITLE: Methods and compositions that affect melanogenesis
INVENTOR(S): Orlow, Seth J.; Hall, Andrea; Manga, Prashiela
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U. S.
Ser. No. 599,487.

APPLICANT

CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002034772	A1	20020321	US 2001-827428	20010406
WO 2002098347	A2	20021212	WO 2002-US11067	20020408
WO 2002098347	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1383474	A2	20040128	EP 2002-776548	20020408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529975	T	20040930	JP 2003-501389	20020408
TW 235659	B	20050711	TW 2002-91107018	20020408
US 2004175767	A1	20040909	US 2004-758335	20040115
US 2006188953	A1	20060824	US 2006-408108	20060420
PRIORITY APPLN. INFO.:				
			US 1999-141563P	P 19990629
			US 2000-599487	A2 20000623
			US 2001-827428	A 20010406
			WO 2002-US11067	W 20020408
			US 2004-758335	A3 20040115

AB The invention provides methods of screening for compds. that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacol. and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compds. and pharmacol. compns. useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1969:481610 CAPLUS Full-text
 DOCUMENT NUMBER: 71:81610
 TITLE: Pyrrolidine steroids
 AUTHOR(S): Kocor, Marian; Kroszczynski, Wojciech
 CORPORATE SOURCE: Polska Akad. Nauk, Warsaw, Pol.
 SOURCE: Roczniki Chemii (1969), 43(4), 783-90
 CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal
 LANGUAGE: Polish

GI For diagram(s), see printed CA Issue.

AB Synthesis of new steroid derivs. containing pyrroline or pyrrolidine ring condensed with the D-ring of steroid skeleton was given. Thus, a solution of 7.5 g. 16 α -nitromethyl-5-pregnene-3 β -ol-20-one acetate (I, R = Ac), 6 ml. (CH₂OH)₂ and 0.2 g. p-toluenesulfonic acid in 300 ml. dry C₆H₆ was refluxed 5 days with a Dean-Stark azeotropic trap, washed with 5% aqueous NaHCO₃ and H₂O, and evaporated to give 7.5 g. 16 α -nitromethyl-20-ethylenedioxy-5-pregnen-3 β -ol acetate (II, R = Ac) (III), m. 177-8°, [α]_D 205800 -63° (c 1, CHCl₃). When refluxed 30 min. in 100 ml. MeOH with 10 ml. aqueous solution containing 2 g.

K₂CO₃, then diluted with 100 ml. H₂O and extracted with Et₂O, 2 g. III afforded 1.5 g. II (R = H), m. 170-1° (MeOH and 0.1% pyridine), [α]_D²⁰ +5800 -57° (c 1.1, CHCl₃). A solution of 1 g. II (R = H) in 50 ml. Et₂O or tetrahydrofuran was treated at 0° with 0.6 g. LiAlH₄ in 50 ml. of the above solvent, then refluxed 1 hr., and treated at 0° with 2N NaOH to give 0.55 g. 16α-aminomethyl-20-ethylenedioxy-5-pregnen-3β-ol (IV), m. 161-4° (Et₂O), [α]_D²⁰ +5800 -73° (c 1, CHCl₃). A solution of 2 g. IV in 30 ml. MeOH and a small amount of 2N HCl kept a few hrs., then diluted with H₂O and evaporated gave 1.6 g. 16α-aminomethyl-5-pregnen-3β-ol-20-one (V), acetate m. 164-6°, [α]_D²⁰ +5800 1° (c 1, CHCl₃). Oppenauer oxidation of 2 g. III in 70 ml. PhMe with 15 ml. cyclohexanone and 1 g. Al(OPr-iso)₃ in 20 ml. PhMe afforded 1.3 g. 16α-nitromethyl-20-ethylenedioxy-4-pregnen-3-one (VI), m. 146-8° (MeOH and 0.1% C₅H₅N), [α]_D²⁰ +5800 36° (c 1, CHCl₃). Acid hydrolysis of VI, or oxidation according to Oppenauer of I (R = H) led to 16α-nitromethylprogesterone (VII), m. 146-8°, [α]_D²⁰ +5800 145° (c 1, CHCl₃). Ketalization of 1 g. VII yielded 66% 16α-nitromethyl-3,20-bis(ethylenedioxy)-5-pregnene (VIII), m. 235-8°, [α]_D²⁰ +5800 -51° (c 1.9, CHCl₃). Reduction of 1 g. VIII with LiAlH₄ gave 0.65 g. 16α-aminomethyl-3,20-bis(ethylenedioxy)-5-pregnene (IX), m. 207-10°, [α]_D²⁰ +5800 -58° (c 1, CHCl₃). A solution of 1 g. V.HCl in 50 ml. tert-BuOH and 2 g. tert-BuOK was refluxed 10 hrs., diluted with 50 ml. H₂O and extracted with C₆H₆. The extract was evaporated and the dry residue chromatographed on Al₂O₃ and eluted with C₆H₆-CHCl₃ to give 0.52 g. 3β-hydroxy-5-androsteno[17,16-c]-2-methyl-1-pyrroline (X), m. 243-5°, [α]_D²⁰ +5800 -114° (c 1.1, CHCl₃). Oppenauer oxidation of 1 g. X gave 0.25 g. 3-oxo-4-androsteno[17,16-c]-2-methyl-1-pyrroline (XI), m. 168-9°, [α]_D²⁰ +5800 28° (c 1, CHCl₃). When acetylated, XI yielded almost quant. 16α-(acetamidomethyl)-17-iso-5-pregnen-3β-ol-20-one acetate, m. 186-8° (aqueous MeOH), [α]_D²⁰ +5800 128° (c 1.1, CHCl₃). A solution of 1 g. X.HClO₄ in 50 ml. MeOH was treated with 0.4 g. NaBH₄ in 20 ml. MeOH, stirred 1 hr. at room temperature, diluted with H₂O and evaporated. The residue was subjected to countercurrent extraction with 1:1:1 C₆H₆-MeOH-H₂O to give 340 mg. 3β-hydroxy-5-androsteno[17,16-c]-2-methylpyrrolidine (XII), m. 209-11° (MeOH), [α]_D²⁰ +5800 -75° (c 1.1, CHCl₃).

L4 ANSWER 3 OF 3 USPATFULL on STN

ACCESSION NUMBER: 2002:60938 USPATFULL Full-text *APPLICANT*
 TITLE: Methods and compositions that affect melanogenesis
 INVENTOR(S): Orlow, Seth J., New York, NY, UNITED STATES
 Hall, Andrea, New York, NY, UNITED STATES
 Manga, Prashiela, New York, NY, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002034772	A1	20020321
APPLICATION INFO.:	US 2001-827428	A1	20010406 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-599487, filed on 23 Jun 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-141563P	19990629 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ANN-LOUISE KERNER, PH.D., HALE AND DORR LLP, 60 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	92	
EXEMPLARY CLAIM:	1	

NUMBER OF DRAWINGS: 19 Drawing Page(s)

LINE COUNT: 4216

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides methods of screening for compounds that affect melanogenesis and the function of P protein in organisms, cells, or cell-free systems. The invention further relates to pharmacologic and cosmetic uses of methods of inhibiting melanogenesis, methods of activating melanogenesis, and compounds and pharmacologic compositions useful for the inhibition or activation of melanogenesis and, therefore, for lightening or darkening the pigmentation of cells and tissue, i.e., skin.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d his

(FILE 'HOME' ENTERED AT 10:13:11 ON 08 JAN 2007)

FILE 'REGISTRY' ENTERED AT 10:13:25 ON 08 JAN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 EXA FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 10:14:14 ON 08 JAN 2007

L4 3 S L3

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

14.59

75.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.56

-1.56

STN INTERNATIONAL LOGOFF AT 10:16:22 ON 08 JAN 2007

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	8	"3389051"	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2007/01/08 11:13
L2	3	"6749940"	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2007/01/08 11:13
L3	2	"6749840"	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2007/01/08 11:13
S1	1506	"progesterone".clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:11
S2	11078	"topical".clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:11
S3	118	S1 and S2	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:15
S4	1266	"phenothiazine".clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:15
S5	20	S2 and S4	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:17

EAST Search History

S6	487	(trifluoperazine or chlorpromazine or prochlorperazine).clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:18
S7	43	S2 and S6	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:25
S8	361	"sphingosine".clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:25
S9	22	S2 and S8	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:27
S10	487	(imipramine or nortriptyline or protriptyline or trimipramine or doxepin).clm.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:28
S11	39	S2 and S10	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:38
S12	3	UK204042	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	OFF	2006/12/29 16:38